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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 4	DEC 18	CA/CAplus patent kind codes updated
NEWS 5	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 6	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 7	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS 8	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 9	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 10	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 11	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 12	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 13	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 14	JAN 29	PHAR reloaded with new search and display fields
NEWS 15	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 17	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 18	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 19	FEB 26	MEDLINE reloaded with enhancements
NEWS 20	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 21	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 22	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 23	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 24	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 25	MAR 16	CASREACT coverage extended
NEWS 26	MAR 20	MARPAT now updated daily
NEWS 27	MAR 22	LWPI reloaded
NEWS 28	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 29	MAR 30	INPADOCDB will replace INPADOC on STN
NEWS 30	APR 02	JICST-EPLUS removed from database clusters and STN

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

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FILE 'HOME' ENTERED AT 13:28:36 ON 10 APR 2007

=> FILE REG

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:29:00 ON 10 APR 2007
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STRUCTURE FILE UPDATES: 9 APR 2007 HIGHEST RN 929600-10-2
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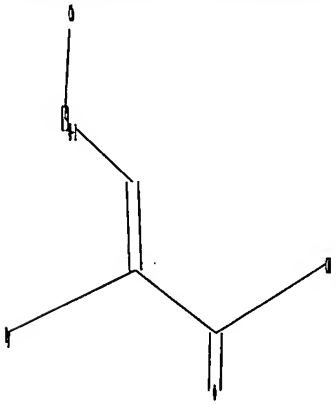
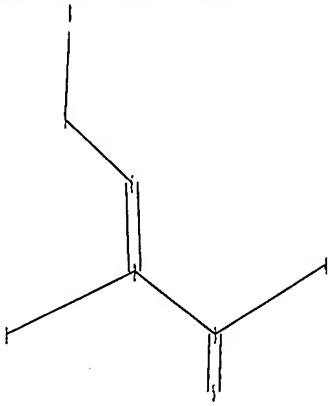
Uploading C:\Program Files\Stnexp\Queries\10776559.str



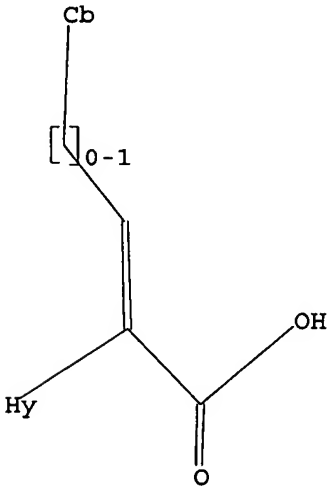


chain nodes :
1 2 3 4 5 6 7 8
chain bonds :
1-2 2-3 2-6 3-4 3-5 6-7 7-8
exact/norm bonds :
1-2
exact bonds :
2-3 2-6 6-7 7-8
normalized bonds :
3-4 3-5

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom

L1 STRUCTURE UPLOADED

=> D
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1
SAMPLE SEARCH INITIATED 13:29:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14758 TO ITERATE

13.6% PROCESSED 2000 ITERATIONS 5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 287883 TO 302437
PROJECTED ANSWERS: 373 TO 1101

L2 5 SEA SSS SAM L1

=> S L1 FULL
FULL SEARCH INITIATED 13:29:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 296925 TO ITERATE

100.0% PROCESSED 296925 ITERATIONS 769 ANSWERS
SEARCH TIME: 00.00.03

L3 769 SEA SSS FUL L1

=> FILE CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 13:29:46 ON 10 APR 2007
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FILE COVERS 1907 - 10 Apr 2007 VOL 146 ISS 16
FILE LAST UPDATED: 9 Apr 2007 (20070409/ED)

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=> S L3
L4 256 L3

=> D L4 230-256 IBIB ABS HITSTR TOT

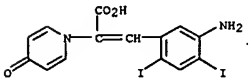
L4 ANSWER 230 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:2241 CAPLUS
DOCUMENT NUMBER: 54:2241
ORIGINAL REFERENCE NO.: 54:530d-i,531a-c
TITLE: Isonicotinoylacetic ester and its derivatives. II. Condensation with aldehydes and amines
AUTHOR(S): Magidson, O. Yu.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Sci. Research Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 165-74
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:2241

AB cf. C.A. 50, 16764c. To 9.7 g. Et isonicotinoylacetate in 20 ml. EtOH there was added at 10° 2 ml. formalin and after 3 hrs. the mixture was heated 4 hrs. on a steam bath, concentrated in vacuo and heated 3 hrs. with 10 ml. 6N HCl; after neutralization with 30% NaOH, there separated 78% 1,3-diisonicotinoylpropane (I), m. 92-3°; mono-HCl salt, decomposing 254-6°; di-HCl salt is very soluble; dioxime, m. 197-8° (80% EtOH). Heating 3 g. I with 2 g. HONH2.HCl and 10 ml. 90% EtOH in a sealed tube 7 hrs. at 160° gave 38% 2,6-bis(4-pyridyl)pyridine, HCl salt tetrahydrate, m. 280-5°; free base, m. 144-6° (EtOAc). The infrared spectrum of the substance is shown. The free base also forms a very soluble di-HCl salt and a picrate, decomposing 252-4°. Reduction of I with (iso-PrO)3Al-iso-PrOH 4 hrs. on a steam bath gave after the usual treatment 82% glassy 1,5-di(4-pyridyl)pentanediol, b0.5 242-5°. Heating 7.7 g. Et isonicotinoylacetate with 3 g. m-O2NC6H4CHO in 5 ml. EtOH 4 hrs. with slow distillation of the solvent gave, after an aqueous treatment and refluxing the product 3 hrs. with 5:3 HCl, 1,3-diisonicotinoyl-2-(m-nitrophenyl)propane, m. 151-2° (MeOH); dioxime, m. 258-60°. Heating 9.7 g. Et isonicotinoylacetate with 5.8 g. BzH and 1 drop piperidine 3 hrs. on a steam bath gave after treatment with 5% HCl, followed by 10% NaOH, α,α'-diisonicotinoyl-β-phenylglutaric acid di-Et ester (II), m. 102-3°, and Et benzyli deneisonicotinoylacetate (III), m. 110-12°, separated by crystallization from 70% MeOH. The former refluxed with 20% HCl gave 2-phenyl-1,3-diisonicotinoylpropane, m. 103° (monohydrate), m. 108-10° (anhydrous). An attempt to form the oxime of II gave 3-(4-pyridyl)isoxazolone, decomposing 194-5°, which also formed in a similar attempt made with III. Condensation of Et isonicotinoylacetate (IV) with salicylaldehyde in EtOH gave a little isonicotinoylacetylisonicotinoylacetic acid, m. 261-2°. A mixture of 9.6 g. IV with 8.3 g. CCl3CHO.H2O gave after 3 hrs. on a steam bath with 10 ml. AcOH and after dilution with 10 ml. H2O after cooling, a solid mass which was extracted with EtOAc to give 4-C5H4NCOCH(CHOHCCl3)CO2Et, m. 139-41° (EtOAc); this, heated with 20% HCl gave γ-pyridyl 3,3,3-trichloro-2-hydroxypropyl ketone, m. 177-8°, and a small amount of a substance, m. 307-10°, which was not identified. Heating 9.5 g. I with 3.7 g. p-Me2NC6H4CHO in 5 ml. AcOH 4 hrs. at 120° gave 3.3 g. yellow 2,5-diisonicotinoyl-3-(p-dimethylaminophenyl)glutaric acid

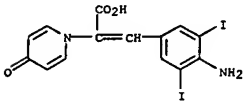
L4 ANSWER 230 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
di-Et ester, m. 137-8°. Heating 8.6 g. o-C6H4(NH2)2 and 15.4 g. I in xylene to 145-50° with gradual distn. of low boiling materials gave 15.5 g. 2-benzimidazolylmethyl γ-pyridyl ketone, m. 211-12°; HCl salt, m. 230-5°. Hydrogenation of 9.5 g. m-nitro-p-anisidine in EtOH over Pt at normal pressure, rapid filtration and treatment of the filtrate with 11.5 g. I, followed by addn. of 40 ml. xylene and heating to 150° with slow distn. gave a solid, which was extd. with MeOH at reflux; the cooled ext. gave a yellow ppt. while the filtrate on acidification with HCl and kept 2 days gave a ppt. which was taken up in hot 5% HCl and treated with AcONa to yield a red ppt.; this treated with NH4OH gave 3 g. yellow 2[4(5)-methoxybenzimidazolyl]methyl 4-pyridyl ketone, m. 317-19° (C5H5N); di-HCl salt, yellow, m. 275-7°. Refluxed with 48% HBr 5 hrs. this gave yellow-green 2-[4(5)-hydroxybenzimidazolyl]methyl 4-pyridyl ketone tri-HBr salt, does not m. 370°; the mother liquor gave more of this product which treated with H2O gave red mono-HBr salt; treated with NaOH this gave a yellow solid of the free base, does not m. 370°.

IT 106652-52-2P, 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- 106652-69-1P, 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 106652-52-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-69-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

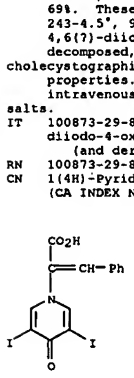


L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:2240 CAPLUS
DOCUMENT NUMBER: 54:2240
ORIGINAL REFERENCE NO.: 54:530a-d
TITLE: Studies on the chemistry of radiopaque compounds. I. α-[N-(4-Pyridonyl)]cinnamic acids and their iodo derivatives
AUTHOR(S): Bojarska-Dahlig, Halina
CORPORATE SOURCE: Inst. Farmaceutyczny, Warsaw
SOURCE: Roczniki Chemii (1959), 33, 589-603
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The following α-[N-(4-pyridonyl)]- (I) and α-[N-(3,5-diiodo-4-pyridonyl)]cinnamic acids (II) were prepared by the reaction of benzaldehyde (III) or substituted III with Na salts of 4-pyridone-N-acetic acid (IV) or 3,5-diiodo derivative of IV in presence of excess of acetic anhydride at 140-50° (modified Perkin synthesis) (compound, m.p., and % yield given): I, 271-2°, 54; I 3-nitro derivative (V), 208-9°, 92; I 3-methoxy derivative, 375.5-8.5°, 55; I 3-hydroxy derivative, 249.5-51°, 66; I 4-nitro derivative (VI), 279.5-80.5°, 73; I 4-methoxy derivative, 276-8°, 53; I 4-hydroxy derivative, 251.5-2.5°, 44; I 2-chloro derivative, 217-18°, 65; II, 278-80°, 77; II 3-nitro derivative (VII), 281.5-2.5°, 95; II 4-nitro derivative (VIII), decomposed, 74; II 4-methoxy derivative, 266-7°, 67; II 2-chloro derivative, 254-5°, 84. All the compds. melted with decomposition V, VI, VII and VIII were reduced to the amino derivs.: 281-2°, 92%; 243-4°, 88%; decomposed, 82%; and 266.5°, 69%. These were iodinated by ICl to give: 4,6(?)-diiodo-3-amino, 243-4.5°, 98; 3,5-diiodo-4-amino derivs. of I, decomposed, 97; 4,6(?)-diiodo-3-amino, 289-91°, 99; 3-iodo-4-amino derivs. of II, decomposed, 96. The iodo derivs. were tested on dogs for cholecystographic properties. The results were neg. on administration per os, but pos. on intravenous administration of aqueous solns. of their N-methylglucamine salts.

IT 100873-29-8, 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo-
(and derivs.)

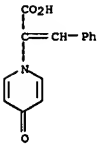
RN 100873-29-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



IT 100725-76-6, 1(4H)-Pyridineacetic acid, α-benzylidene-4-oxo-

L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(and iodine-contg. derivs.)

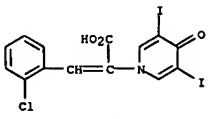
RN 100725-76-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-benzylidene-4-oxo- (6CI) (CA INDEX NAME)



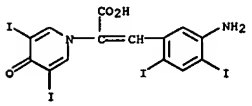
IT 100540-95-2P, 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- 100541-48-8P, 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- 100873-32-3P, 1(4H)-Pyridineacetic acid, α-(4-amino-3-iodobenzylidene)-3,5-diiodo-4-oxo- 100961-30-6P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- 101094-71-7P, 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-4-oxo- 101278-67-5P, 1(4H)-Pyridineacetic acid, α-(5-acetamido-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- 106590-29-8P, 1(4H)-Pyridineacetic acid, α-p-nitrobenzylidene-4-oxo- 106590-61-8P, 1(4H)-Pyridineacetic acid, α-m-nitrobenzylidene-4-oxo- 106652-51-1P, 1(4H)-Pyridineacetic acid, α-[p-aminobenzylidene]-3,5-diiodo-4-oxo- 106652-52-2P, 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- 106652-68-0P, 1(4H)-Pyridineacetic acid, α-[m-aminobenzylidene]-3,5-diiodo-4-oxo- 106652-69-1P, 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo- 106782-71-2P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-nitrobenzylidene-4-oxo- 106783-04-4P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-m-nitrobenzylidene-4-oxo- 107558-27-0P, 1(4H)-Pyridineacetic acid, α-p-hydroxybenzylidene-4-oxo- 107558-89-4P, 1(4H)-Pyridineacetic acid, α-m-hydroxybenzylidene-4-oxo- 107920-25-2P, 1(4H)-Pyridineacetic acid, α-[p-aminobenzylidene]-4-oxo- 107922-11-2P, 1(4H)-Pyridineacetic acid, α-[m-aminobenzylidene]-4-oxo- 108620-58-2P, 1(4H)-Pyridineacetic acid, α-p-methoxybenzylidene-4-oxo- 108621-67-6P, 1(4H)-Pyridineacetic acid, α-m-methoxybenzylidene-4-oxo- 860411-11-6P, 1(4H)-Pyridineacetic acid, α-(m-acetamidobenzylidene)-3,5-diiodo-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 100540-95-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

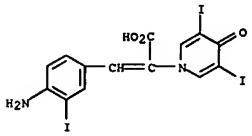
L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



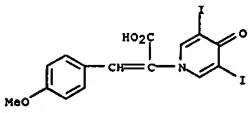
RN 100541-48-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



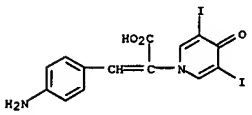
RN 100873-32-3 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-amino-3-iodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



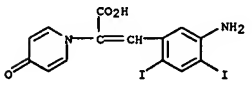
RN 100961-30-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- (6CI) (CA INDEX NAME)



L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 106652-52-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-68-0 CAPLUS
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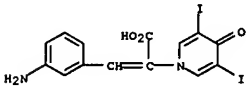
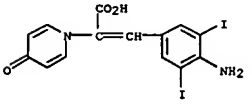


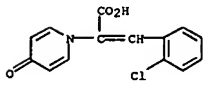
RN 106652-69-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



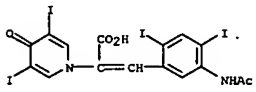
RN 106782-71-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(p-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

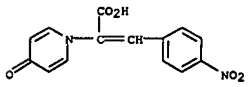
RN 101094-71-7 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-4-oxo- (6CI) (CA INDEX NAME)



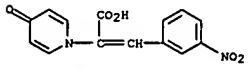
RN 101278-67-5 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-acetamido-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



RN 106590-29-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

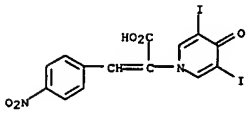


RN 106590-61-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

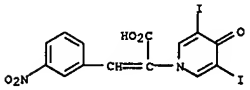


RN 106652-51-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-aminobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

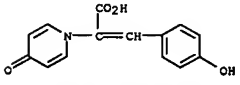
L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



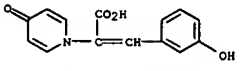
RN 106783-04-4 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(m-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



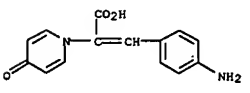
RN 107558-27-0 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-hydroxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



RN 107558-89-4 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-hydroxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

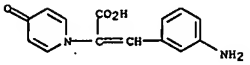


RN 107920-25-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-aminobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

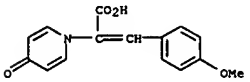


L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

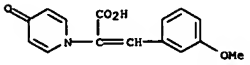
RN 107922-11-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-aminobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



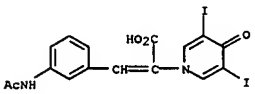
RN 108620-58-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-methoxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



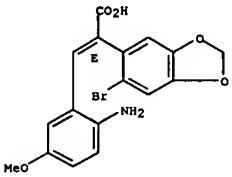
RN 108621-67-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-methoxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



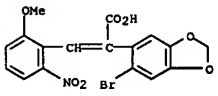
RN 860411-11-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-acetamidobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



L4 ANSWER 232 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 232 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:1971 CAPLUS
DOCUMENT NUMBER: 54:1971
ORIGINAL REFERENCE NO.: 54:401f-h
TITLE: 2-Nitro-6-methoxybenzaldehyde
AUTHOR(S): Pettit, Geo. R.
CORPORATE SOURCE: Univ. of Maine, Orono
SOURCE: Journal of Organic Chemistry (1959), 24, 866-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The synthesis of trans-2-amino-6-methoxy-α-(3,4-methylenedioxy-6-bromophenyl)cinnamic acid (I) from 2-nitro-6-methoxybenzaldehyde (II) was described. 2-Methyl-3-nitrophenol (73 g.) in 400 ml. H2O containing 19. g.
NaOH was treated with 60 g. Me2SO4, heated 2 hrs. on the steam bath, and the crude mixture steam distilled to give 42 g. 2-nitro-6-methoxytoluene (III),
m. 55-7.5°. III (40 g.) in 250 ml. CS2 added during 0.5 hr. to 70 g. chromyl chloride in 150 ml. CS2, left 72 hrs. at room temperature, the solid
immediately collected, washed, the solid added to H2O, and extracted with CHCl3 gave 15 g. II, m. 110-11° (CCl4), λ 5.85 μ. II (2 g.), 3.06 g. 6-bromohomopiperonylic acid, 10 ml. Ac2O, and 1 ml. NEt3 was refluxed 15 min. to give 0.87 g. 2-nitro analog (IV) of I, yellow crystals, m. 264-5° (decomposition), λ 5.95 μ. IV (0.55 g.)
in 3.3 g. FeSO4, 0.2 ml. HCl, and 5 ml. H2O heated to 90-5° before addition of 3 ml. 28% NH4OH, the mixture heated a further 45 min., filtered
hot, and the filtrate acidified gave 0.41 g. I, m. 205-6° (MeOH-H2O), λ 5.95 μ.
IT 130862-09-8P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)- 876659-16-4P, Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans-
RL: PREP (Preparation)
(preparation of)
RN 130862-09-8 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)- (6CI) (CA INDEX NAME)



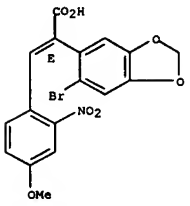
RN 876659-16-4 CAPLUS
CN Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:72502 CAPLUS
DOCUMENT NUMBER: 53:72502
ORIGINAL REFERENCE NO.: 53:13124a-g
TITLE: Phenanthrene derivatives. II. Synthesis of 3-methoxy-5,6(and 6,7)-methylenedioxyphenanthrene
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi
CORPORATE SOURCE: Nagoya City Univ.
SOURCE: Yakugaku Zasshi (1959), 79, 245-8
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Na homopiperonylate (I) (5.8 g.), 5.2 g. 2,4-O2N(MeO)C6H3CHO (II), and 25 ml. Ac2O heated 20 hrs. at 120°, heated 30 min. with 50 ml. H2O, the AcOH removed in vacuo, the residue taken up in 500 ml. 5% NH4OH, washed with Et2O, and the solution acidified with HCl yielded 6.8 g. trans-α-(3,4-methylenedioxyphenyl)-2-nitro-4-methoxycinnamic acid (III), columns, m. 212-13° (EtOH), and the mother liquor gave 0.5 g. cis-isomer (IV) of III, m. 237°. FeSO4.7H2O (4.4 g.) in 10 ml. H2O and 12 ml. concentrated NH4OH treated dropwise with 1 g. III in 20 ml. 5%
NH4OH, heated 10 min. on a H2O bath, the solution filtered, and the filtrate
treated with HCl to pH 5 gave 0.8 g. 2-NH2 analog (V) of III, granules, m.
202-3° (decomposition) (EtOH). Similarly, 0.5 g. IV yielded 0.3 g. 3-(3,4-methylenedioxyphenyl)-7-methoxycarbostyril (VI), needles, m. 272°. Or, 0.8 g. V in 50 ml. pure EtOH refluxed 2 hrs., and the solution concentrated gave 0.6 g. VI, m. 272° (EtOH). V (1 g.) in 40 ml. MeOH and 12.5 ml. 20% H2SO4 at 0° diazotized with 10 ml. N NaNO2, kept 30 min., 15 ml. H2O added, 3 g. Cu added portionwise, stirred until the evolution of N ceased, heated 30 min. on a H2O bath, the solution made
alkaline with NH4OH, concentrated, and the product extracted with Et2O gave 0.3 g.
3-methoxy-6,7-methylenedioxy-9-phenanthrenecarboxylic acid (VII), needles,
m. 324-5° (decomposition) (EtOH); the mother liquor concentrated gave 0.05 g.
5,6-CH2O2 analog (VIII) of VII, needles, m. 266-8° (decomposition). 6,3,4-Br(CH2O2)C6H2CH2CO2Na (2.8 g.), 1.8 g. II, and 20 ml. Ac2O treated as in III gave 2.8 g. trans-α-(2-bromo-4,5-methylenedioxyphenyl)-2-nitro-4-methoxycinnamic acid (IX), granules, m. 204°. FeSO4.7H2O (13.2 g.) in 30 ml. H2O and 36 ml. concentrated NH4OH treated with 2 g. IX in 40
ml. 5% NH4OH and the product treated as in V yielded 1.3 g. 2-NH2 analog (X) of IX, granules, m. 207-8° (decomposition). X (1.3 g.) in 24 ml. MeOH and 15 ml. 20% H2SO4 diazotized with 12 ml. N NaNO2 gave 0.4 g. 1-bromo-3,4-methylenedioxy-6-methoxy-10-phenanthrenecarboxylic acid (XI). X (1 g.) in 20 ml. EtOH refluxed 10 hrs. and cooled gave 0.5 g. 3-(2-bromo-4,5-methylenedioxyphenyl)-7-methoxycarbostyril (XII), needles, m. 284-5°. Catalytic reduction of 0.4 g. IX in 40 ml. EtOH and 40 ml. 10% KOH-EtOH with 0.3 g. Pd-C yielded 0.2 g. VIII, m. 266-8° (decomposition). VIII (0.2 g.) in 10 ml. C9H7N and 0.2 g. Cu heated 10 min. at
180-200° and 20 min. at 250-60°, cooled, Et2O added, washed with dilute HCl, neutralized with 5% NaOH, the Et2O removed, and the residue
in C6H6 passed through Al2O3 gave 0.06 g. 3-methoxy-5,6-methylenedioxyphenanthrene (XIII), needles, m. 134° (EtOH);

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
picrate, needles, m. 172-3° (decompn.). Similarly 0.1 g. VII as above yielded 0.02 g. 6,7-CH2O2 analog of XIII, needles, m. 135-6°; picrate m. 161-2° (decompn.).
IT 130862-01-0P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(4-methoxy-2-nitrophenyl)-, trans- 876659-18-6P, Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- 876659-46-0P, Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)-, trans- 876659-64-2P, Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- 876659-65-3P, Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, cis-
RL: PREP (Preparation)
(preparation of)
RN 130862-01-0 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(4-methoxy-2-nitrophenyl)-, trans- (6CI) (CA INDEX NAME)

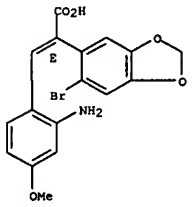
Double bond geometry as shown.



RN 876659-18-6 CAPLUS
CN Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

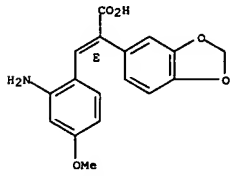
Double bond geometry as shown.

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 876659-46-0 CAPLUS
CN Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

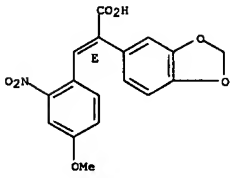
Double bond geometry as shown.



RN 876659-64-2 CAPLUS
CN Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

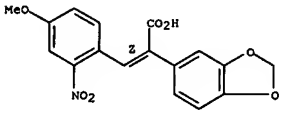
Double bond geometry as shown.

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 876659-65-3 CAPLUS
CN Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, cis- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



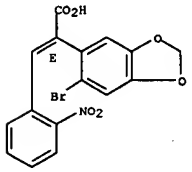
L4 ANSWER 234 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:72501 CAPLUS
DOCUMENT NUMBER: 53:72501
ORIGINAL REFERENCE NO.: 53:13123d-i,13124a-b
TITLE: Phenanthrene derivatives. I. Synthesis of 3,4-methylenedioxyphenanthrene
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi
CORPORATE SOURCE: Nagoya City Univ.
SOURCE: Yakugaku Zasshi (1959), 79, 241-4
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 3,4-CH2O2C6H3CH2CO2Na (I) (6.7 g.), 5 g. 2-O2NC6H4CHO, and 33 ml. Ac2O heated 20 hrs. at 120°, the product heated 30 min. with 50 ml. H2O, the AcOH removed in vacuo, the residue treated with 500 ml. 5% NH4OH, washed with Et2O, and the solution acidified with HCl gave 4.2 g. trans-2-O2NC6H4CH:C(C6H3O2CH2-3,4)CO2H (II), columns, m. 224-5° (EtOH); the mother liquor concentrated gave 1.4 g. cis analog (III) of II,
columns, m. 192-3°. FeSO4.7H2O (4.4 g.) in 10 ml. H2O and 12 ml. concentrated NH4OH treated dropwise with 1 g. II in 20 ml. 5% NH4OH, heated 10
min. on a H2O bath, the solution filtered while hot, and the filtrate treated
with concentrated HCl to pH 5 gave 0.8 g. 2-NH2 analog (IV) of II, granules, m.
208° (decomposition) (EtOH). Similarly, 0.5 g. III yielded 0.3 g. 3-(3,4-methylenedioxyphenyl)carbostyril (V), needles, m. 256-7°. Or, 1 g. IV, 10 ml. Ac2O, and 1 ml. concentrated H2SO4 heated 30 min. at 100°, cooled, heated 30 min. with 50 ml. H2O, and the solution neutralized with NaHCO3 yielded 0.7 g. V, needles, m. 256-7° (EtOH). IV (1 g.) in 20 ml. MeOH and 12.5 ml. 20% H2SO4 at 0° diazotized with 10 ml. N NaNO2, kept 30 min., the solution with 15 ml. H2O
treated portionwise with 3 g. Cu, stirred until the evolution of N ceased,
made alkaline with NH4OH, the solution concentrated, the residue acidified with HCl,
and the product extracted with Et2O gave 0.38 g. 2,3-methylenedioxy-10-phenanthrenecarboxylic acid (VI), needles, m. 212-13° (decomposition) (EtOH); the mother liquor concentrated gave 0.02 g. 3,4-CH2O2 analog (VII) of
VI, needles, m. 267° (decomposition). VI (0.12 g.) in 10 ml. C9H7N and 0.2 g. Cu heated 10 min. at 180-200° and 20 min. at 250-60°, the solution diluted with Et2O, washed with dilute HCl, neutralized with 5% NaOH,
the Et2O removed, and the residue in C6H6 passed through Al2O3 gave 0.06 g. 2,3-methylenedioxyphenanthrene (IX), columns, m. 93-4°; picrate m. 151-2° (EtOH). Similarly, 0.1 g. VII yielded 0.03 g. 3,4-methylenedioxyphenanthrene (X), columns, m. 70-1°; picrate, red brown needles, m. 168° (decomposition). The free acid (18 g.) of I in 200 ml. CHCl3 treated dropwise with 16 g. Br at 10-15°, kept 2 hrs., and the product recrystd. (C6H6) gave 20.2 g. 6,3,4-Br(CH2O2)C6H2CH2CO2H (XI), needles, m. 190°. Na salt (10.4 g.) of XI, 5.6 g. 2-O2NC6H4CHO, and 35 ml. Ac2O treated as in II gave 9.4 g. trans-α-(2-bromo-4,5-methylenedioxyphenyl)-2-nitrocinnamic acid (XII), columns, m. 237°. FeSO4.7H2O (6.6 g.) in 15 ml. H2O and 18 ml. concentrated NH4OH treated dropwise with 1 g. XII in 20 ml. 5% NH4OH and the
product treated as in IV yielded 0.7 g. 2-NH2 analog (XIII) of XII,

L4 ANSWER 234 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
granules, m. 223°. XIII (1 g.) in 10 ml. Ac2O and 1 ml. concd. H2SO4 gave product which treated as for V yielded 0.7 g. 3-(2-bromo-4,5-methylenedioxyphenyl)carbostyril (XIV), granules, m. 279-80°. XIII (2.4 g.) in 48 ml. MeOH and 30 ml. 20% H2SO4 diazotized with 24 ml. N NaNO2 gave 0.8 g. 1-bromo-3,4-methylenedioxy-10-phenanthrenecarboxylic acid (XV). Reducing 0.2 g. XV in 20 ml. EtOH and 20 ml. 10% KOH-EtOH with 0.2 g. Pd-C, concg. the soln., extg. the residue with H2O, acidifying with HCl, and extg. with Et2O gave 0.11 g. VII, needles, m. 267° (decompn.). VII (0.2 g.) in 20 ml. C9H7N treated with 0.3 g. Cu as in X yielded 0.05 g. X, m. 70-1°; picrate m. 168° (decompn.).

IT 131410-39-4P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- 132727-18-5P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, cis- 132727-19-6P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- 876659-42-6P, Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- 876659-44-8P, Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans-
RL: PREP (Preparation)
(preparation of)

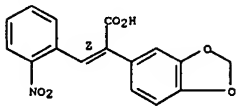
RN 131410-39-4 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 132727-18-5 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, cis- (6CI) (CA INDEX NAME)

Double bond geometry as shown.

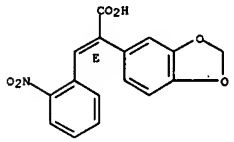


L4 ANSWER 234 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 234 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

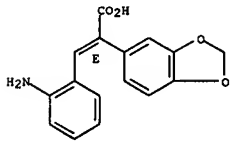
RN 132727-19-6 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



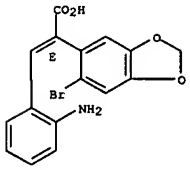
RN 876659-42-6 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 876659-44-8 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 235 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:62535 CAPLUS
DOCUMENT NUMBER: 53:62535
ORIGINAL REFERENCE NO.: 53:11325i,11326a-i,11327a-f
TITLE: Plant substances containing a nitro group. III. The synthesis of a degradation product of aristolochic acid-II, 3,4-methylenedioxy-10-acetamidophenanthrene
AUTHOR(S): Pailer, M.; Schleppnik, A.
SOURCE: Monatshefte fuer Chemie (1958), 89, 175-85
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:62535

AB cf. C.A. 52, 1979e. Aristolochic acid-II, obtained from Aristolochia clematitis, previously (loc. cit.) identified as 3,4-methylenedioxy-10-nitrophenanthrene-1-carboxylic acid, has been degraded by decarboxylation, acetylation, and reduction, to 3,4-methylenedioxy-10-acetamidophenanthrene (I). Piperonylidenerhodanine (II) was obtained in 93% yield when 60 g. piperonal and 51 g. rhodanine in 800 ml. boiling AcOH was treated with 200 g. anhydrous AcONa, stirred 30 min. at boiling, cooled, and poured into 4 l. H2O. The crystals were washed with water and dried at 110° to yield 94 g. II, m. 294°. β-(3,4-Methylenedioxyphenyl)-α-thiopyruvic acid (III), was prepared by suspending 108 g. II in 620 ml. 15% NaOH, heating on the water bath with occasional stirring until solution was complete, filtering, cooling to -5°, and adding 670 ml. 10% HCl. After 1 hr. at -5°, filtering and washing with H2O, and drying in vacuo, III was obtained in quant. yield (crude), m. 221-5° (decomposition) (AcOH-H2O). β-(3,4-Methylenedioxyphenyl)pyruvic acid oxime (IV) was obtained when 84 g. NH2OH.HCl in concentrated aqueous solution was poured into a solution of 27.5g. Na in 800 ml. EtOH, the NaCl filtered off, the filtrate added to 79.5 g. III, and warmed on the water bath until H2S evolution stopped. The solvent was evaporated in vacuo, the residue dissolved in 575 ml. 5% NaOH, filtered, cooled at 0°, and stirred with 600 ml. 10% HCl. The yellow, crystalline powder was filtered off, washed with water, and dried in vacuo over KOH to yield 76 g. (crude) IV, m. 159-61° (decomposition) (dilute EtOH). Homopiperonylic acid (V) was obtained when 62 g. IV was suspended in 240 ml. Ac2O, warmed carefully under reflux to completion of the reaction, and 15 min. further to boiling, and the excess Ac2O removed in vacuo to produce V nitrile, a red-brown oil, which was immediately saponified with 42 g. KOH in 75 ml. H2O and 300 ml. MeOH for 6 hrs. to give 28.5 g. V, m. 126-8°. V (24.8 g.) treated with 22 g. Br in 150 ml. glacial AcOH gave 35.9 g. 6-bromohomopiperonylic acid (VI), m. 190-1°. VI (27.5 g.), 15.1 g. o-nitrobenzaldehyde, 11.0 g. NEt3, and 100 ml. Ac2O heated 6 hrs. at 100° gave 32.3 g. α-(3,4-methylenedioxy-6-bromophenyl)-2-nitrocinnamic acid (VII), m. 238-9° (EtOH). VII (32.3 g.) in 300 ml. H2O and 80 ml. concentrated NH4OH was reduced in a mixture of 200 g. FeSO4.7H2O, 380 ml. H2O, and 140 ml. concentrated NH4OH to 26.2 g. VII 2-NH2

L4 ANSWER 235 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
analog (VIII), citron-yellow, m. 226-7° (decompn.) (EtOH). VIII (26.2 g.) in 300 ml. dioxane was treated with cooling and vigorous stirring with 6 ml. concd. H2SO4 and 12 ml. iso-AmONO, stirred 30 min., and the ppt. dissolved in 100 ml. H2O; 150 ml. 50% H3PO2 was quickly added, the soln. stirred, and poured into 1 l. H2O. The ppt. was filtered off, boiled with dil. Na2CO3 soln., filtered, acidified, and the ppt. filtered off and recrystd. several times from glacial AcOH to yield 9.6 g. 1-bromo-3,4-methylenedioxyphenanthrene-10-carboxylic acid (IX), m. 233-5° (decompn.). IX (8.0 g.) in 25 g. KOH and 350 ml. 50% EtOH was heated to boiling and 9 g. Zn dust added. After boiling 3 hrs., filtering, evapg. EtOH, acidifying with 1:1 HCl, filtering, and washing with H2O, the yellow ppt. was dried in vacuo at 110° to yield 6.2 g. 3,4-methylenedioxyphenanthrene-10-carboxylic acid (X), after vacuum sublimation at 150°, m. 274-5°, also prepd. by Pschorr ring closure of VIII; X with CH2N2 gave X Me ester (XI), m. 126° (MeOH). XI (900 mg.) and 5.1 ml. N2H4.H2O in 10 ml. dioxane and 20 ml. MeOH boiled 3 hrs. gave X hydrazide (XII), m. 248-52° (MeOH). XII (700 mg.) was dissolved in 20 ml. dioxane with warming, then cooled in ice water, and treated with 3.5 ml. concd. HCl, and then with 0.4 ml. iso-AmONO to give X azide (XIII), m. 91° (decompn.). XIII (475 mg.) boiled 3 hrs. in toluene freshly distd. over Na gave 3,4-methylenedioxy-10-phenanthryl isocyanate (XIV), not isolated, but boiled 1 hr. with 1 ml. Ac2O, then evapd. in vacuo, the residue dissolved in C6H6, heated with C, filtered, and treated with petr. ether until the turbidity disappeared. On cooling, 170 mg. of a mixt. sepd., m. 174-81°. The mixt. was distd. at 180°/0.001 mm. and the yellow oil crystd. several times from MeOH to give a substance, m. 255-6°, not identified. The MeOH soln. was evapd., and the residue again distd. at 180°/0.001 mm. to yield after two sublimations, 5 mg. 3,4-methylenedioxy-10-acetamidophenanthrene (XV), m. 274° which gave no m.p. depression when mixed with I. A stirred mixt. of 648 mg. X, 2 ml. CF3CO2H, and 2 ml. (CF3CO)2O, was treated with abs. CHCl3 until the soln. was clear, then with 200 mg. NaN3 to form a jelly, which was dild. with 20 ml. petr. ether, filtered off, washed with petr. ether, and dried in vacuo. The product was boiled with Et2O and evapd. to dryness quickly under N. The residue (XVI) (35 mg.), after distn. at 130°/0.001 mm., m. 153-4°, and was believed to be the amine from XV. The amine (XVII) obtained directly from I m. 154-5°. Both XVI and XVII, when diazotized, gave a violet-brown dye with alk. β-naphthol soln. XVI (20 mg.) in 2 ml. Ac2O, boiled 5 min. gave 11 mg. N-Ac compd., m. 274-5° (as did XV), no m.p. depression with I, m. 274°. The ultraviolet spectra were [location of max. in λ (log ε)]: I, 248 (4.61), 281 (3.91), 297 (3.72), 313 (3.87), 323 (3.85), 350 (3.34), 368 (3.30); XV, 248 (4.54), 282 (4.05), 298 (3.77), 314 (3.95), 324 (3.94), 350 (3.42), 368 (3.39). The infrared spectra of both I and XV in perfluorokerosine suspension gave a strong band at 3220 cm.-1, indicating the NH group, and thus the monoacetylamino group. V (4.5 g.), 3.8 g. o-nitrobenzaldehyde (XVIII), 2.5 g. NEt3, and 25 g. Ac2O heated 6 hrs. at 100°, treated carefully with 100 ml. H2O with addnl. warming, and cooled gave a resinous product, from which the liquid was

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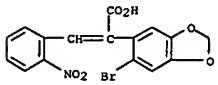
decanted. The resin was dissolved in NH4OH, filtered, acidified with 1:1 HCl with stirring, the crude acid filtered off, washed with H2O, and crystd. from AcOH to yield 4.6 g. α-(3,4-methylenedioxyphenyl)-2-nitrocinnamic acid (XIX), yellow crystals, m. 226-8° (EtOH). XIX (4.2 g.) was heated with 70 ml. H2O and 10 ml. NH4OH soln., added with stirring to 30 g. FeSO4.7H2O, 20 ml. NH4OH soln., and 200 ml. H2O on the water bath, stirred 30 min., filtered, and washed with hot H2O to give 2.4 g. yellow α-(3,4-methylenedioxyphenyl)-2-aminocinnamic acid (XX), m. 209-10°. XX (2.3 g.) in 40 ml. dioxane cooled 1 ml. concd. H2SO4 then 2 ml. iso-AmONO added dropwise with stirring, stirred 30 min., treated with 10 ml. H2O, then added quickly to 20 ml. 50% H3PO2 + Cu powder gave a white flocculent ppt. The mixt., free from diazonium salt, was poured into 100 ml. H2O, filtered, the ppt. digested with 1% KOH, filtered, washed with H2O, and dried in vacuo at 110° to yield 2.2 g. of an acid mixt., which, boiled with AcOH, recrystd. several times from HCONMe2, and sublimed at 210°/0.001 mm. gave an unidentified acid (XXI), m. 328-9°. From the mother liquor crude X was sepd. From the filtrate an acid was obtained in small amt., m. 219-21°, not identified. XXI (50 mg.) suspended in 50 ml. boiling AcOH, treated with a soln. of 100 mg. Na2Cr2O7 in 1 ml. H2O and 10 ml. AcOH, poured into 200 ml. H2O, extd. with CHCl3, the CHCl3 soln. washed with H2O, 1% KOH, and H2O, dried with Na2SO4, and evapd. yielded a red mass which was distd. at 186°/0.001 mm. The dark red compd. crystd. twice from AcOH and sublimed several times gave 8 mg. 2,3-methylenedioxy-9,10-phenanthrenequinone (XXII), m. 253°. The acid XXI was thus 2,3-methylenedioxyphenanthrene-10-carboxylic acid. XXI (50 mg.) decarboxylated with 50 mg. naturkupfer C in 5 ml. freshly distd. quinoline at 220° yielded, after crystn. from MeOH and distn. at 100°/0.001 mm., 2,3-methylenedioxyphenanthrene, leaflets, m. 93-5°; picrate m. 152°.

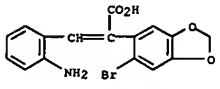
IT 131410-38-3P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)- 132569-41-6P, Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- 132727-17-4P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- 857176-14-8P, Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)-
RL: PREP (Preparation)
(preparation of)

RN 131410-38-3 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)- (6CI) (CA INDEX NAME)

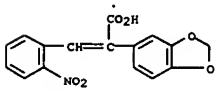


L4 ANSWER 235 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

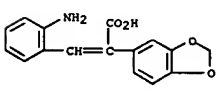
RN 132569-41-6 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 132727-17-4 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- (6CI) (CA INDEX NAME)



RN 857176-14-8 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



L4 ANSWER 236 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1959:50945 CAPLUS
DOCUMENT NUMBER: 53:50945
ORIGINAL REFERENCE NO.: 53:9129i,9130a-g
TITLE: Revision of structural assignments for geometrical isomers of 3-methyl-5-phenylpentadienoic acid
AUTHOR(S): Wiley, Richard H.
CORPORATE SOURCE: Imp. Coll. Sci. & Technol., London
SOURCE: Journal of the Chemical Society (1958) 3831-8
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Reinvestigation of the geometrical isomers of PhCH:CHCMe: CHCO2H (I) has shown that the compound, m. 125°, formerly assigned the cis-2-trans-4-structure is a mol. complex of the isomers, m. 158° and 160°. On the basis of their phys. properties and their infrared and ultraviolet absorption characteristics, these 2 isomers are now assigned the cis-2-trans-4- (Ia) and the trans-2-trans-4-structure (Ib), resp. This reassignment makes possible a new interpretation of the steric course of the Reformatskii reaction and of the mechanism of the decarboxylation by which the isomers are prepared, as well as the clarification of several inconsistencies and apparent abnormalities previously noted. In the Reformatskii reaction of PhCH:CHAc with BrCH2CO2Et the reaction was repeated on a 0.14-molal basis by the procedure previously given (Cawley and Nelan, C.A. 50, 4788i), giving a 1st fraction of 1.4 g. crystals, m. 124-52°, and 2.6 g., m. 124-6°. Recrystn. of the former gave Ib, m. 159-60°. The mol. complex purified by recrystn. from ligroine, or ligroine with 5% C6H6, m. 125-6°. Et senecioate and N-bromosuccinimide gave Me2CBrCH:CHCO2Et (II), n24D 1.4995. II by the Reformatskii reaction with BzH gave 15.14 g. unsatd. ester which was separated into 8 fractions, b3 115°/3 mm. to 166°/1.5 mm. The 7th fraction, b1.5 160-6°, was treated with saturated alc. KOH; acidification of the Et2O-extracted, diluted reaction mixture gave a solid which on recrystn. yielded 0.8 g. Ia, m. 158-8.5°. Further cooling of the mother liquor gave a 2nd and 3rd fraction. Recrystn. of the 2nd fraction gave 0.1 g. of the complex of Ia and Ib. The infrared spectra for 4 of the ester fractions showed a band at 1764 cm.-1, indicative of a γ-lactone. Attempts to isolate a γ-lactone by more careful fractionation were unsuccessful. Ia was obtained by the following procedure. The lutidine solution was not evaporated before being poured into dilute aqueous acid to precipitate the crude product.

HO2CC(:CHPh)CMe:CHCO2H (III) (7.10 g.) gave 3.55 g. Ia. III di-K salt warmed with AcOH and the Et2O solution of the neutral fraction evaporated gave a fraction, b3-5 76-81°, m. 33-5°, λ 218, 225, 232, and 282 mμ, ε 17,850, 17,400, 11,300, and 41,800, which may be PhCH:CHCMe:CH2. The infrared absorption spectrum shows a prominent band at 962 cm.-1, characteristic of the trans-disubstituted ethylenes. Either Ia or Ib, obtained by decarboxylation, or the mol. complex, when treated with iodine gave Ib. The mother liquors from the isomerization of Ib gave the mol. complex. Samples of Ib obtained from the iodine-catalyzed isomerization and Ib obtained by decarboxylation were used for the phase diagram. The 50% composition point is not a simple, single eutectic point.

The existence of a maximum in the curve is not clearly shown by the available

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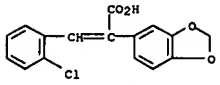
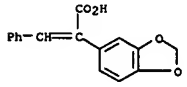
data. A mixt. of 0.6005 g. each of Ia and Ib fused together and recrystd.
gave the mol. complex, m. 125-6°. The infrared absorption spectrum for this sample is identical with, and superimposable on, that of the complex obtained from the Reformatskii reaction with benzylideneacetate. The complex may also be formed by recrystn. of equal amts. of Ia and Ib. Ia (0.93 g.) with CH2N2 in Et2O gave 0.67 g. of the Me ester (IV), m. 41.5-2.5° (ligroine), λ 232, 238, and 312 mμ, ε 14,350, 11,500, and 28,300. Similarly Ib (0.45 g.) with ethereal CH2N2 gave 0.41 g. Me ester (V), m. 35-6° (ligroine), λ 308, 238, and 232 mμ, 37,600, 9900, and 11,900. A mixt. of IV and V liquefied at room temp. Methylation of the mol. complex gave a mixt. of IV and V which, when cooled to -78°, pptd. crystals. The liquid residue, after thorough evacuation, was analyzed and had λ 310, 238, and 232 mμ, ε 32,000, 10,600, and 13,800. The infrared absorption spectra of the acids were detd. as Nujol mulls and those of the esters as liquid films.

IT 109697-83-8P, Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- 877169-81-8P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 109697-83-8 CAPLUS
CN Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 877169-81-8 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl- (6CI) (CA INDEX NAME)



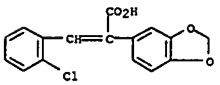
L4 ANSWER 237 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:50944 CAPLUS
DOCUMENT NUMBER: 53:50944
ORIGINAL REFERENCE NO.: 53:9129d-i
TITLE: The synthesis of α-(o-nitroaryl)cinnamic acids
AUTHOR(S): Pailer, M.; Schleppnik, A.; Meller, A.
SOURCE: Monatshefte fuer Chemie (1958), 89, 211-19
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The Perkin reaction of 1 mol. o- or p-nitroaryl acetic acids (I) with 1 mol. aromatic aldehyde was carried out in good yields in 1000 ml. Ac2O (II) 24 hrs. at the low temperature of 50-60° in the presence of 1.1 mols. Et3N as catalyst to give α-aryl cinnamic acids as intermediates for 3-arylidenoxindoles and phenanthrene carboxylic acids. The low reactivity of I in the Perkin reaction previously reported results from the ease of decarboxylation at higher temps. and is also a consequence of the mesomeric and inductive effects of the substituents on the acid and carbonyl reactants. The products were isolated from the condensation reaction by (A): adding 2-3 vols. H2O, boiling, cooling, decanting the H2O, digesting the oil or resin in dilute NH4OH on the steam bath, decolorizing with animal C, acidifying the filtrate with 5N HCl and recrystg. the precipitated nitrocinnamic acid; (B): adding 2-3 vols. cold H2O to decompose II and recrystg. the condensation product. With o-O2NC6H4CH2CO2H (III) (aldehyde, isolation method, yield and m.p. given): PhCHO (IV), A, 42, 193-4° (alc.); p-MeC6H4CHO, B, 37, 187° (HOAc); MeOC6H4CHO (V), A, 42, 172-3° (MeOH); (MeO)2C6H3CHO, A, 40, 158-9° (C6H6); piperonal (VI), A, 27, 226-7° (MeOH); 6-allylpiperonal, A, 25, 211-12° (HOAc); vanillin, B, 12, 196-7° (alc.); o-vanillin, B, 23, 204-5° (HOAc); o-HOC6H4CHO (VII), B, 32, α-(o-O2NC6H4)-2-acetoxy-3-methoxycinnamic acid 176-7° (HOAc); o-ClC2H4CHO (VIII), B, 77, 3-(2-nitrophenyl)-coumarin, 225° (HOAc); p-ClC6H4CHO, B, 70, 210-11° (HOAc); 6-bromopiperonal (IX), A, 55, 261-2° (HOAc) (at a reaction temperature of 30°, evolution of CO2 from decomposition of III and IX recovered unchanged); 6-bromoveratraldehyde, B, 57, 229-31° (HOAc); o-O2NC6H4CHO (X), A, 65, 207° (HOAc); m-O2NC6H4CHO, A, 96, 200-1° (alc.); 2,5-MeOO2NC6H3CHO, B, 38, 225-6°, (HOAc); 6-nitropiperonal, B, 78, 261° (HOAc); 2-nitroveratraldehyde, A, 68, 244° (HOAc); 6-nitroveratraldehyde, A, 66, 247° (HOAc); 3,4-(HO)2C6H3CHO, -, 0, -; 2,4-(OH)2C6H3CHO, -, 0, -; o-HO2CC6H4CHO, -, 0, -; p-Me2NC6H4CHO, -, 0, -. With p-O2NC6H4CH2CO2H: IV, A, 38, 225-6° (HOAc); V, B, 10, 244-5° (MeOH); X, A, 62, 185-6° (HOAc); VII, B, 26, 266-8°, (HOAc); VI, -, 0, -. With homopiperonylic acid (aldehyde and yield given): IV, 32; X, 62% (at a reaction temperature of 100°, 78% yield and at 125°, 38% yield); VIII, 51.

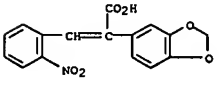
IT 109697-83-8P, Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- 132727-17-4P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- 877169-81-8P,

L4 ANSWER 237 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl-
RL: PREP (Preparation)
(prepn. of)

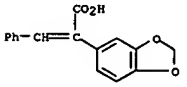
RN 109697-83-8 CAPLUS
CN Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 132727-17-4 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- (6CI) (CA INDEX NAME)



RN 877169-81-8 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl- (6CI) (CA INDEX NAME)

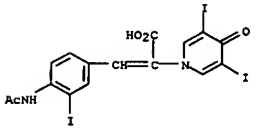


L4 ANSWER 238 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:2693 CAPLUS
DOCUMENT NUMBER: 53:2693
ORIGINAL REFERENCE NO.: 53:530d-g
TITLE: The relation between electrical resting potential of the isolated perfused mammalian muscle and the extracellular potassium concentration
AUTHOR(S): Pillat, B.; Kraupp, O.; Giebisch, G.; Stormann, H.
CORPORATE SOURCE: Univ. Vienna
SOURCE: Pfluegers Archiv fuer die Gesamte Physiologie des Menschen und der Tiere (1958), 266, 459-72
CODEN: AGPPAS; ISSN: 0365-267X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

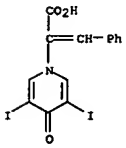
AB The resting potential (I) of the gracilus muscle, the mechanical tension (II) developed by the gastrocnemius muscle, the blood flow (III) and the lactic acid outflow (IV) of the isolated hindleg of the cat were determined, first with normal extracellular K concentration, then with increased K concentration, both at a constant product of K and Cl concentration (V) and at a constant Cl concentration At constant V the I was decreased by increased K concentration There was a linear relation between the decrease of I and the log of the K concentration At constant Cl concentration the same linear relation existed. The slopes of the two lines differed significantly. Both lines could be derived theoretically by assuming a Donnan equilibrium for K+ and Cl- on either side of the membrane. No changes in the II corresponding to the changes in the I could be found. Increase of the K concentration decreased the III strongly in both cases. A complete stop of the flow occurred at K concns. above 50 millimoles/l. No spontaneous increase of the IV occurred during the increase of the K concentration Due to the lowered III, the IV increased continually during the high K concentration

IT 101727-17-7P, 1(4H)-Pyridineacetic acid, α-(4-acetamido-3-iodobenzylidene)-3,5-diiodo-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 101727-17-7 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-acetamido-3-iodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

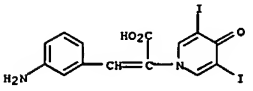


L4 ANSWER 239 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:61176 CAPLUS
DOCUMENT NUMBER: 52:61176
ORIGINAL REFERENCE NO.: 52:11037h-i,11038a
TITLE: α-[N-(3,5-Diiodo-4-pyridonyl)]cinnamic acids and their derivatives
AUTHOR(S): Bojarska-Dahlig, Halina
CORPORATE SOURCE: Inst. Farm., Warsaw
SOURCE: Roczniki Chemii (1957), 31, 1333-4
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A modified Perkin reaction between the respective aldehydes, Ac2O, and the Na salt of 3,5-diiodo-4-pyridone-N-acetic acid gave α-[N-(3,5-diiodo-4-pyridonyl)]cinnamic acid (I), m. 275-6°, and the following derivs. of I (m.ps. given): o-Cl (II), 251.5-2.5°; p-MeO (III), 271.5-3°; m-NO2 (IV), 276.5-8°, and p-NO2 (V), decompose IV and V were reduced to the corresponding NH2 derivs., (VI), m. 269.5-71°, and (VII), m. 263-4°, resp. Iodination of VI and VII with I2Cl in dilute HCl gave the respective amino iodocinnamic acids (VIII), m. 277.5-9.5°, and (IX), decompose 270°. III showed lowest toxicity in mice. Cholecystographic properties were studied on dogs and it was shown that I, VIII, and IX do not collect in the gall-bladder but are eliminated through the alimentary canal.
IT 100873-29-8, 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo-
(and derivs.)
RN 100873-29-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

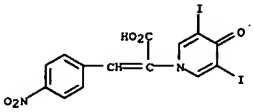


IT 100540-95-2P, 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- 100961-30-6P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- 106652-51-1P, 1(4H)-Pyridineacetic acid, α-[p-aminobenzylidene]-3,5-diiodo-4-oxo- 106652-68-0P, 1(4H)-Pyridineacetic acid, α-[m-aminobenzylidene]-3,5-diiodo-4-oxo- 106782-71-2P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-nitrobenzylidene-4-oxo- 106783-04-4P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-m-nitrobenzylidene-4-oxo-
RL: PREP (Preparation)

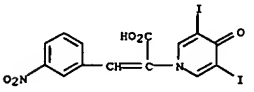
L4 ANSWER 239 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



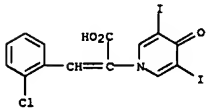
RN 106782-71-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(p-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



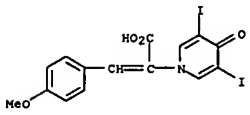
RN 106783-04-4 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(m-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



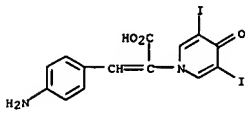
L4 ANSWER 239 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (prepn. of)
RN 100540-95-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



RN 100961-30-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-51-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-aminobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-68-0 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-aminobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

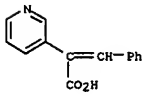
L4 ANSWER 240 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:55905 CAPLUS
DOCUMENT NUMBER: 52:55905
ORIGINAL REFERENCE NO.: 52:10078b-i,10079a-c
TITLE: N-Oxides and related compounds. VII. Peracid oxidation of some conjugated pyridines
AUTHOR(S): Katritzky, A. R.; Monro, A. M.
CORPORATE SOURCE: Oxford Univ., UK
SOURCE: Journal of the Chemical Society (1958) 150-3
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 52, 4633d. β-3- and β-4-Pyridylacrylic acids and their ethyl esters and amides, 2- and 4-styrylpyridines and pyridine-2-aldoxime and its semicarbazone gave 1-oxides with AcO2H. Pyridine (0.01 mole), 1.47 ml. 30% aqueous H2O2, and 6 ml. AcOH was heated 18 hrs. at 70°, volatile matter removed at 100°/15 mm., the residue either crystallized directly, or if semisolid treated in 15 ml. hot CHCl3 with 0.8 g. K2CO3 and recovered from the CHCl3 by evaporation The following 1-oxides were prepared: β-4-pyridylacrylic, prisms, m. 237-40° (AmOH) (decomposition), hemiacetate, plates, m. 237-40° (AcOH) (decomposition); β-4-pyridylacrylamide, prisms, m. 246° (MeOH or H2O) (decomposition); Et β-4-pyridylacrylate, prisms, m. 145° (C6H6-petr. ether), which with 2N aqueous NaOH during 12 hrs. at 100° followed by AcOH gave the corresponding acid, m. 238-40° (decomposition), and with aqueous methanolic NH3 in 5 days at 0° gave the amide, m. 245° (decomposition); β-3-pyridylacrylic acid, prisms m. 273-4° (AcOH) (decomposition); β-3-pyridylacrylamide, needles, m. 235° (EtOH-H2O) (decomposition); Et β-3-pyridylacrylate, prisms, m. 99-101° (AcOEt), also prepared by esterification of the corresponding acid with EtOH-H2SO4, converted (as in the 4-series) into the acid, m. 274-5° (decomposition), and the amide, m. 235° (decomposition). Oxidation gave the oxide of the 2-isomer as prisms, m. 162° (C6H6), and the 4-isomer gave an oxide, prisms, m. 169° (MeCOEt). BzH (10.6 g.), 10.9 g. 2-picoline 1-oxide, and 50 ml. 5% KOMe in MeOH was refluxed 3 hrs., after 12 hrs. more, excess CO2 was passed in, the whole filtered and steam distilled yielding 22% 2-styrylpyridine 1-oxide, m. 160°. 4-Picoline 1-oxide similarly gave 11% 4-styrylpyridine 1-oxide, m. 167-9°. Refluxing 20.4 g. Et 3-pyridylacetate 8 hrs. with 11 g. KOH in 11 ml. H2O and 28 ml. EtOH followed by addition of 14.6 ml. aqueous 12N HCl, filtration, evaporation, and extraction of the residue with MeOH gave 75% 3-pyridylacetic acid, m. 141-3°; 1-oxide, prisms, m. 142-4° (AcOEt-EtOH) (decomposition). The acid (1.27 g.), 1.5 ml. BzH, 0.2 ml. piperidine, and 10 ml. pyridine heated 2 days at 115° and poured into H2O gave 40% β-phenyl-α-3-pyridylacrylic acid, needles, m. 234-5° (EtOH) (decomposition). Aqueous 10% NaOH (0.5 ml.) was added slowly at 0° to 1.07 g. pyridine-2-aldehyde and 1.17 g. PhCH2CN in 2.0 ml. EtOH; after 18 hrs. 74% α-phenyl-β-2-pyridylacrylonitrile was collected as prisms, m. 63-6° (EtOH). O-Benzoyl(pyridine-2-aldehyde cyanohydrin), prepared as the oxime benzoate below, formed prisms, m. 102° (EtOH). Pyridoin, needles, m. 156°, separated later from the aqueous mother liquors. Aqueous NaCN (0.94 g. in 2 ml.) was added slowly at -10° to 3.14 g. quinoline-2-aldehyde in 10 ml. aqueous 2N HCl and the precipitated solid recrystd. (C6H6 and AcOEt) to

L4 ANSWER 240 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
give 62% 1-cyano-1,2-di(2-quinolyl)-ethane-1,2-diol, brown plates, m. 133° (decompn.). v Oxidation gave the aldoxime oxide, needles, m. 222° (EtOH) (decompn.); semicarbazone oxide, insol. in CHCl3, needles, m. 233° (AcOH-AcOEt) (decompn.). Both compds. with 2,4-dinitrophenylhydrazine in alc. HCl gave the corresponding 2,4-dinitrophenylhydrazone 1-oxide, needles, m. 285-90° (AcOH) (decompn.). Extn. of crude pyridine-2-aldehyde cis-semicarbazone 1-oxide with CHCl3 gave (from the CHCl3) 3% cis-semicarbazone, prisms, m. 158° (EtOH). On treatment with alc. HCl and 2,4-dinitrophenylhydrazine, both the cis- and normal semicarbazones gave the 2,4-dinitrophenylhydrazone, m. 226-8°. BzCl (0.32 ml.) was added slowly to 0.31 g. pyridine-2-aldoxime in 1 ml. pyridine at 0°, the mixt. kept 18 hrs., and H2O added yielding 80% O-benzoyl(pyridine-2-aldoxime), prisms, m. 85-90° (EtOH). Treatment with AcO2H gave BzOH and pyridoin, m. 152°. 4-Acetylpyridine gave the azine, plates, m. 125.5-7° (petr. ether), and when heated 1 min. with 2 parts hydrazine hydrate yielded the hydrazone, plates, m. 121-2° (C6H6). Oxidation of 2-, 3-, and
4-(N'-benzenesulfonylhydrazinocarbonyl)p
yridine gave the 4-substituted pyridine 1-oxide, needles, m. 238-9° (H2O) (decompn.), the 3-analog, needles, m. 222-4° (H2O or EtOH) (decompn.), and the 2-analog, needles, m. 209-12° (AcOH) (decompn.). Et isonicotinate (5.5 g.) was refluxed 4 hrs. with 12 ml. PhCH2NH2 and excess amine removed at 100°/14 mm. yielding 71% N-benzylisonicotinamide, needles, m. 90-2° (AcOEt-petr. ether); the methotoluene-p-sulfonate formed plates, m. 194.5-6.5° (EtOH). N-2-(3-Indoyl)ethylisonicotinamide, m. 165.5-67°, was similarly prepd. by heating the amine and ester for 10 hrs. at 140° and sepg. from EtOH-C6H6; methotoluene-p-sulfonate, plates, m. 174-5.5° (AcOEt-EtOH). Oxidation gave pure β-4-pyridylpropionamide 1-oxide, rods, m. 227° (EtOH), and N-benzylisonicotinamide 1-oxide, prisms, m. 184° (EtOH).

IT 32967-19-4P, 3-Pyridineacetic acid, α-benzylidene-
RL: PREP (Preparation)
(preparation of)

RN 32967-19-4 CAPLUS

CN 3-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



L4 ANSWER 241 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:35138 CAPLUS

DOCUMENT NUMBER: 52:35138

ORIGINAL REFERENCE NO.: 52:6298f-i,6299a-b

TITLE: Synthesis of 1-methoxy-5,6-methylenedioxyphenanthrene

AUTHOR(S): Shirai, Hideaki; Oda, Noriichi; Toyonaka, Keiko

CORPORATE SOURCE: Nagoya City Univ. Pharm. School

SOURCE: Nagoya-shiritsu Daigaku Yakugakubu Kiyo (1957), 5, 58-60
CODEN: NADYAS; ISSN: 0469-4805

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

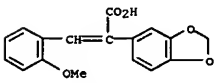
AB Na 6-bromohomopiperonylate, 2.2 g. 2-methoxy-6-nitrobenzaldehyde, and 20 cc. Ac2O is heated at 120° 32 hrs., 40 cc. H2O added, heated on a steam bath 30 min., the AcOH vacuum distilled, 200 cc. 5% NH4OH added, filtered, the filtrate shaken with ether to remove impurities, acidified with HCl, extracted with EtOAc, and the product recrystd. from MeOH to afford
3.2 g. 2-methoxy-6-nitro-α-(3,4-methylenedioxy-6-bromophenyl)cinnamic acid (I), light yellow columns, m. 260-1° (decomposition). I (1.5 g.) in 15 cc. 5% NH4OH is added dropwise to 9 g. FeSO4, 22 cc. H2O, and 20 cc. concentrated NH4OH with shaking, warmed on a steam
bath 20 min., filtered, the filtrate adjusted to pH 5.0 by dilute HCl, and
the precipitate recrystd. from C6H6 to afford 1.0 g.
2-methoxy-6-amino-α-
(3,4-methylenedioxy-6-bromophenyl)cinnamic acid (II), light yellow needles, m. 202-3°. To 0.3 g. II in 7 cc. MeOH is added 4.3 cc. 20% H2SO4, cooled at 0°, diazotized with 3 cc. N NaNO2 solution, kept 30 min., 3 cc. H2O added, 0.3 g. Gatterman's mol. Cu added with shaking, heated on a steam bath 1 hr., made alkaline by NH4OH, the Cu removed, the filtrate evaporated in vacuo, acidified with HCl, the precipitate extracted with ether,
and recrystd. from MeOH to afford 0.06 g. 1-bromo-3,4-methylenedioxy-8-methoxyphenanthrene-10-carboxylic acid (III), m. 265-85°. III (0.06 g.) in 60 cc. alc. is reduced using 30 cc. 10% KOH-alc. and 0.2 g. Pd-C as catalyst, evaporated in vacuo, dissolved in 15 cc. H2O, acidified with
HCl, extracted with ether, and recrystd. from MeOH to afford 0.04 g. 1-methoxy-5,6-methylenedioxyphenanthrene-9-carboxylic acid (IV), light yellow needles, m. 269-70°. IV (0.04 g.) and 0.2 g. Gatterman's mol. Cu in 5 cc. quinoline is heated at 180-200° 10 min., then boiled 250-60° 20 min., cooled, diluted with ether, Cu removed, the ether layer shaken with dilute HCl to remove quinoline, shaken with 2% NaOH
solution to remove unreacted IV, the ether evaporated, the residue dissolved in
C6H6, chromatographed on an alumina column, and recrystd. from MeOH to afford 0.01 g. 1-methoxy-6,6-methylenedioxyphenanthrene (V), columns, m. 87-8°; picrate, reddish brown needles from alc., m. 180° (decomposition). 2-Methoxy-α-(3,4-methylenedioxyphenyl)cinnamic acid (VI) was also prepared Na homopiperonylate (0.5 g.) and o-methoxybenzaldehyde in 5 cc. Ac2O is heated at 110-20° 10 hrs., 10 cc. H2O added, heated on a steam bath 30 min., the AcOH evaporated in

L4 ANSWER 241 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
vacuo, 30 cc. 5% NH4OH added, filtered, the filtrate shaken with ether to remove the unreacted compds., acidified with HCl, and recrystd. from dil. AcOH to afford 0.9 g. VI, light yellow needles, m. 219-20°.

IT 87751-89-1P, Acrylic acid, 3-(o-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- 111089-64-6P, Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- 130862-09-8P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)-
RL: PREP (Preparation)
(preparation of)

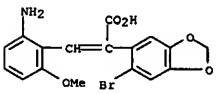
RN 87751-89-1 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



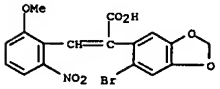
RN 111089-64-6 CAPLUS

CN Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 130862-09-8 CAPLUS

CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)- (6CI) (CA INDEX NAME)



L4 ANSWER 242 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1957:51904 CAPLUS

DOCUMENT NUMBER: 51:51904

ORIGINAL REFERENCE NO.: 51:9646b-f

TITLE: Alkaloids of menispermaceous plants. CXLIII. Alkaloids
of Stephania capitata. 5

AUTHOR(S): Shirai, Hideaki; Oda, Noriichi

CORPORATE SOURCE: Nagoya City Univ.

SOURCE: Yakugaku Zasshi (1956), 76, 1287-9
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

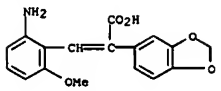
AB cf. C.A. 46, 125d; 51, 1542i. A mixture of 5 g. 3,4-CH2O2C6H3CH2CO2 Na, 4.5
g. 2,6-MeO(O2N)C6H3CHO, and 25 ml. Ac2O heated 20 hrs. at 110-20°, the product boiled with 50 ml. H2O, the AcOH removed in vacuo, the residue
in 300 ml. 5% NH4OH filtered, the filtrate washed with Et2O, the aqueous layer
acidified with HCl, the precipitate taken up in AcOEt, the AcOEt removed, and the
residue recrystd. from MeOH gave 4.5 g. 2,6-MeO(O2N) C6H3CH:C(C6H3O2CH2-3,4)CO2H (I), needles, m. 206-7°; 4.4 g. FeSO4 in 10 ml. H2O and 12 ml. NH4OH treated dropwise with 1 g. I in 20 ml. 5% NH4OH, heated 10 min. at 100°, the solution filtered, and the filtrate treated with HCl to pH 5 gave 0.8 g. 6-NH2 analog (II) of I, m. 107-9° (decomposition); recrystn. of II in MeOH converted into 5-methoxy-3-(3,4-methylenedioxyphenyl)carbostyril, needles, m. 267-8°; 2 g. II in 40 ml. MeOH and 25 ml. 20% H2SO4 at 0° treated dropwise with 20 ml. 1N NaNO2, let stand 30 min., 30 ml. H2O added, heated 30 min. with 10 g. Cu, the solution made alkaline with NH4OH, the Cu and MeOH removed, and the residue
extracted with Et2O gave 0.2 g.
1-methoxy-6,7-methylenedioxyphenanthrene-9-
carboxylic acid (III), light yellow needles, m. 300-1° (decomposition), and the mother liquor concentrated gave 0.15 g. 5,6-CH2O2 analog (IV) of III, m.
267-8°; 0.15 g. IV in 10 ml. C9H7N heated 10 min. with 0.5 g. Cu at 180-200° and 20 min. at 250-60, the solution filtered, the filtrate with Et2O washed with dilute HCl and NaOH, the oil b0.1 210-20° further purified through Al2O3 gave 0.03 g. 1-methoxy-5,6-methylenedioxyphenanthrene (V), columns, m. 86-7° [picrate, m. 180° (decomposition)]. Similarly, III yielded 1-methoxy-6,7-methylenedioxyphenanthrene, prisms, m. 150°; picrate, m. 192-3°(decomposition). Thus, the structure of stephane is confirmed to be 1-methoxy-5,6-methylenedioxyaporphine.

IT 110394-33-7P, Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- 111529-61-4P, Acrylic acid, 3-(2-methoxy-6-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-
RL: PREP (Preparation)
(preparation of)

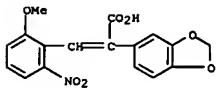
RN 110394-33-7 CAPLUS

CN Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)

L4 ANSWER 242 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 111529-61-4 CAPLUS
CN Acrylic acid, 3-(2-methoxy-6-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-(6CI) (CA INDEX NAME)



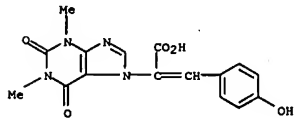
L4 ANSWER 243 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:9499 CAPLUS
DOCUMENT NUMBER: 51:9499
ORIGINAL REFERENCE NO.: 51:2025f-h
TITLE: 7-Theophyllineacetic acid derivatives
INVENTOR(S): Schlesinger, Albert; Weiner, Nathan; Gordon, Samuel M.
PATENT ASSIGNEE(S): Endo Laboratories Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2712016		19550628	US 1952-292194	19520606

AB [Y in this abstract = 7-theophyllinyl]. The Na salt of 7-theophyllineacetic acid (416 g.) (anhydrous), 1200 g. Ac2O, and 192 g. HOC6H4CHO refluxed with stirring about 24 hrs. at 110-12°, the Ac2O and AcOH evaporated in vacuo, the residue stirred with 800 g. H2O and 100 g. ice until it dissolves, 40% NaOH added until alkaline to phenolphthalein, then 200 ml. excess, the mixture heated to 65° with stirring on a water bath, held at room temperature 2 hrs., filtered through glass wool, and the filtrate poured into 2200 concentrated HCl and 2000 g. ice and kept 24 hrs. in an ice bath ppts. 54% YC(: CHR)CO2H (R = p-HOC6H4), m. 254° (from boiling EtOH). By use of the appropriate materials were prepared 94% YCHRCO2H (R = p-HOC6H4CH2), m. 170°; 86% YCHRCO2H [R = 3,5,4-I2(HO)C6H2CH2] (I), m. 274° (from AcOH); the Na salt of I; and the piperidine salt of I, m. 189°. These derivs. are valuable as bactericides, amebicides, and x-ray contrast agents.

IT 101352-23-2P, Purine-7-acetic acid, 1,2,3,6-tetrahydro-α-p-hydroxybenzylidene-1,3-dimethyl-2,6-dioxo-
RL: PREP (Preparation)
(preparation of)

RN 101352-23-2 CAPLUS
CN Purine-7-acetic acid, 1,2,3,6-tetrahydro-α-p-hydroxybenzylidene-1,3-dimethyl-2,6-dioxo- (6CI) (CA INDEX NAME)

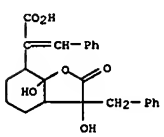


L4 ANSWER 244 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:82002 CAPLUS
DOCUMENT NUMBER: 50:82002
ORIGINAL REFERENCE NO.: 50:15497h-i,15498a-c
TITLE: The condensation of cyclohexanone with phenylpyruvic acid
AUTHOR(S): Kristensen, Johan; Cordier, Paul
SOURCE: Compt. rend. (1956), 242, 908-10
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Aqueous Na-phenylpyruvate (I) with an equimolar amount of cyclohexanone (II) in 3% KOH at 0° for 8 days, then addition of ether, gives 28% of 22,62-diphenyl-21,61-dihydroxy-21,61-dicarboxy-2,6-diethylcyclohexanone (III), m. 285° (semicarbazone, m. 254°; dinitrophenylhydrazone, m. 226°), when purified in HOAc. The ether extract contains 15% of 22-phenyl-21-hydroxy-21-carboxy-2-ethylcyclohexanone (IV), m. 127° obtained by extraction with KHCO3 solution, precipitation with acid, extraction into ether and solvent evaporated, and the crystals triturated with cold C6H6. III and IV decompose in aqueous base to I and II. A large excess of II doubles the yield of IV. III with HCl in HOAc at 100° gives an ethylenic monoacid, m. 118°, possibly V, which gives BzH (VI) with MnO4-and VI and I with hot NaOH. Cold concentrated H2SO4 with III gives the corresponding β-diketone, m. 90°, with loss of H2O and CO. Cold H2SO4 with 1/3 HOAc and III gives the diethylenic diacid, m. 181°, and MnO4- with this compound gives VI and an α,γ-diketo acid. IV with HCl in HOAc at 100° gives VII, m. 91°, and a corresponding ethylenic acid, m. 98°, also obtained with cold H2SO4 and 1/3 HOAc. IV with concentrated H2SO4 gives 1,2,3,4-tetrahydrophenanthrene-10-carboxylic acid, m. 210°. V with KBH4 gives the α,γ-dihydroxy acid, m. 184°, and the corresponding lactone, m. 164°; Raney Ni hydrogenation gives an isomeric lactone, m. 121°. III fails to hydrogenate. A similar condensation with o-methylcyclohexanone (with alc. present) gives only the α-hydroxy-γ-oxo acid, m. 154°.

IT 858791-52-3P, 7-Benzofuranacetic acid, 3-benzyl-α-benzylideneoctahydro-3,7a-dihydroxy-2-oxo-
RL: PREP (Preparation)
(preparation of)

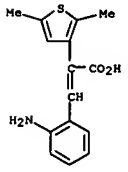
RN 858791-52-3 CAPLUS
CN 7-Benzofuranacetic acid, 3-benzyl-α-benzylideneoctahydro-3,7a-dihydroxy-2-oxo- (5CI) (CA INDEX NAME)



L4 ANSWER 244 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

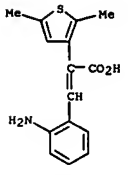
L4 ANSWER 245 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1955:23854 CAPLUS
DOCUMENT NUMBER: 49:23854
ORIGINAL REFERENCE NO.: 49:4619c-i,4620a-b
TITLE: Polynuclear thiophenes. III. 1,3-Dimethyl-4,5-benzisothianaphthene
AUTHOR(S): Dann, Otto; Distler, Harry
CORPORATE SOURCE: Univ. Erlangen, Germany
SOURCE: Chemische Berichte (1954), 87, 365-73
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 49, 1696h. After a discussion of the chemical, phys., and biol. properties of thiophene, naphthalene, and benzene derivs. the preparation of 1,3-dimethyl-4,5-benzisothianaphthene (I) is described and its properties are compared with those of 9,10-dimethyl-1,2-benzanthracene (II). Heating 10 g. 2,5-dimethyl-3-acetylthiophene, 18 cc. dioxane, 22 cc. concentrated NH4OH, 15 g. S, and 12 cc. yellow (NH4)2Sx in a bomb tube 4 hrs. at 160° and evaporating the mixture on a water bath to dryness give 70% (2,5-dimethyl-3-thienyl)acetamide (III), m. 147-8°. Refluxing 10 g. III with 10 g. KOH in 100 cc. MeOH and 5 cc. H2O 12 hrs. gives 54% free acid (IV), m. 68-70°. When 12.7 g. o-O2NC6H4CHO and 12 g. Na salt of IV (dried 6 hrs. at 130°) are refluxed 7 hrs. at 160-70° with 2 g. ZnCl2 in 140 cc. Ac2O, 100 cc. H2O is added carefully to the hot mixture, and the latter is poured into 1 l. H2O 62% 2-nitro-α-(2,5-dimethyl-3-thienyl)cinnamic acid (V), yellow crystals, m. 196°, is obtained. Adding 250 cc. concentrated NH4OH to 110 g. Fe(NH4)2(SO4)2.6H2O in 750 cc. H2O, then adding 10.3 g. V in 100 cc. 10% NH4OH, boiling the mixture 2 hrs. with stirring, and adjusting the filtered solution to pH 5 give 66% 2-NH2 analog (VI) of V, fine needles, m. 215-17°. Adding with stirring 30 g. VI in 400 cc. H2O containing 20 g. KOH to 800 cc. H2O containing 70 cc. H2SO4, then adding (1 hr.) at 0° 25 g. NaNO2 in 150 cc. H2O, stirring the mixture another 4 hrs. at 0-3°, destroying the excess NaNO2 by the addition of 25 g. H2NSO3H in 200 cc. H2O, stirring the solution 5 hrs. with Cu paste [prepared according to Gatterman [Ber. 23, 1219(1890)] from 250 g. crystalline CuSO4], keeping it overnight, filtering off the precipitate, extracting it with dilute NaOH, and acidifying the alkaline solution with dilute H2SO4 give 60-5% crude 1,3-dimethyl-4,5-benzisothianaphthene-7-carboxylic acid (VII) [Me ester (CH2N2), golden-yellow leaflets, m. 226-7° (sealed tube)]. The extracted precipitate is dried overnight at 70°, mixed with some "Naturkupfer C," divided into 3 parts, and each part (about 30 g.) added in 2-3 g. batches to 100 cc. quinoline at 210-20°. The mixture is then heated a very short time to 230° and, after cooling to about

L4 ANSWER 245 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
180°, is poured very slowly into 1 l. H2O contg. 100 cc. concd. H2SO4. The ppt. formed is washed exhaustively with dil. H2SO4 and H2O, suspended in 200 cc. warm Me2CO, 1 l. benzine added to the filtered soln., the amorphous ppt. formed is discarded, the filtered soln. washed (1% H2SO4, 1% NaOH, and H2O), and the dried benzine soln. passed through an Al2O3 column. The yellow zone is eluted with 2 l. benzine (b. 60-70°), the residue of the benzine soln. distd. at 135-40°/4 mm., and the distillate treated in abs. EtOH with picric acid in EtOH, giving I picrate, dark red-brown needles, m. 148-9°, which, decompd. in ether with NaOH and the residue of the ether distd. at 0.4 mm., gives 4% I, needles, m. 82.5-3°. Refluxing 1 g. I in 25 cc. Me2CO with 10 g. maleic anhydride (VIII), pouring the mixt. into 250 cc. H2O contg. 2 g. NaOH, and extg. with ether give 1,4-dimethyl-1,4-endothio-1,2,3,4-tetrahydrophenanthrene-2,3-dicarboxylic anhydride, m. 169-70°, which is also obtained when 50 mg. I and 500 mg. VIII are fused at 160°. Heating 10 g. V mixed with 1 g. Cu chromite in 30 cc. quinoline 0.5 hr. at 230°, pouring the mixt. into dil. H2SO4, extg. with ether, and distg. the residue of the ext. at 205-12°/1.5 mm. give β-(2,5-dimethyl-3-thienyl)-2-nitrostyrene (IX), m. 98-9°. Refluxing 2 g. IX in 25 cc. AcOH and 15 cc. concd. HCl 2 hrs. with 5 g. granulated Zn, distg. the reaction product at 120-60°/0.4 mm., and treating the distillate with HCl give β-(2,5-dimethyl-3-thienyl)-2-aminostyrene-HCl, m. 191-2° (picrate, m. 159-60°). Distg. 60 g. 2-thienylacetamide and 65 g. P2O5 at 216-20° gives 45% 2-thienylacetonitrile (X), b12 105-10°, nD22 1.5436. Refluxing 10 g. X and 20 g. p-MeC6H4SO3H.H2NCH2CH2NH2 1.5 hrs. at 200°, adding dil. NaOH, extg. with CHCl3, and distg. the residue of the CHCl3 ext. give 2-(2-thienylmethyl)imidazoline, b3 166-7°, needles, m. 64-5° (picrate, m. 229-30°).
IT 853919-12-7P, 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl-, hydrochloride 853919-13-8P, 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl- 859795-29-2P, 3-Thiopheneacetic acid, 2,5-dimethyl-α-o-nitrobenzylidene-
RL: PREP (Preparation)
(preparation of)
RN 853919-12-7 CAPLUS
CN 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl-, hydrochloride (5CI) (CA INDEX NAME)

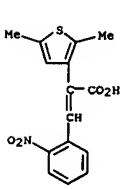


● HCl

RN 853919-13-8 CAPLUS
CN 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl- (5CI) (CA INDEX NAME)

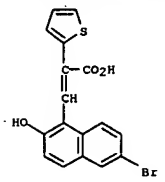


RN 859795-29-2 CAPLUS
CN 3-Thiopheneacetic acid, 2,5-dimethyl-α-o-nitrobenzylidene- (5CI) (CA INDEX NAME)



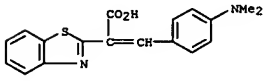
L4 ANSWER 246 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1954:18264 CAPLUS
DOCUMENT NUMBER: 48:18264
ORIGINAL REFERENCE NO.: 48:3327i,3328a-c
TITLE: Derivatives of 6-bromo-2-methoxy-1-naphthaldehyde of biological interest
AUTHOR(S): Hoan, Nguyen
CORPORATE SOURCE: Pharm. fac., Paris
SOURCE: Bulletin de la Societe Chimique de France (1953) 309-14
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:18264
AB A series of 2,3-diarylacrylonitriles and 3-aryl-5,6-benzocoumarins derived from 6-bromo-2-methoxy-1-naphthaldehyde (I) are described. These compds. are being investigated as antagonists of sexual hormones and as inhibitors of plant auxins. I b15 234-40°, m. 110°, from 6,2-BrC10H6OMe, HCONHMe, and POCl3; semicarbazone, m. 246°; thiosemicarbazone (Ia), m. 240°. 6-Bromo-2-methoxy-1-styrylnaphthalene b15 275-80°, m. 101-40° (perhaps a mixture of cis and trans forms), from I and BzMgCl. 6-Bromo-2-methoxy-1-(2,4,6-trinitrostyryl)naphthalene m. 205°, from I and TNT. The following α-(6-Bromo-2-methoxy-1-naphthyl)-β-arylacrylonitriles were prepared (aryl and m.p. given): Ph 159°, p-tolyl 170°, p-EtC6H4 128°, p-ClC6H4, 161°, p-BrC6H4 190°, p-IC6H4 207°, p-O2NC6H4 226°, 2-thienyl 130°, 3-thianaphthenyl 165°. 3-Aryl-5,6-(3-bromobenzo)coumarins (3-aryl and m.p.): Ph 247°, p-tolyl 297°, p-EtC6H4 238°, p-ClC6H4 328°, p-BrC6H4 342°, p-IC6H4 350°, p-O2NC6H4 355°, 2-thienyl 242°, 3-thianaphthenyl 266°. Ia was treated with the following acids to give the corresponding I 4-oxo-2-thiazolin-2-ylhydrazone (II) substituted in the 5 position of the thiazoline nucleus (acid and m.p. of II given): monochloroacetic 305°, α-bromobutyric 229°, α-bromoisovalerianic 237°, α-bromolauric 188°,α-bromomyristic 195°, α-bromopalmitic 184°, α-bromostearic 171°, α-bromodihydrohydnocarpic 169°, α-bromodihydrochaulmoogric 181°.
IT 858200-16-5P, 1-Naphthaleneacrylic acid, 6-bromo-2-hydroxy-α-2-thienyl-, δ-lactone
RL: PREP (Preparation)
(preparation of)
RN 858200-16-5 CAPLUS
CN 1-Naphthaleneacrylic acid, 6-bromo-2-hydroxy-α-2-thienyl-, δ-lactone (5CI) (CA INDEX NAME)

L4 ANSWER 246 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 247 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1953:444 CAPLUS
DOCUMENT NUMBER: 47:444
ORIGINAL REFERENCE NO.: 47:57g-i,58g-i,59a-g
TITLE: Photographic α-substituted carbocyanine sensitizers
AUTHOR(S): van Dormael, A. E.; Nys, J.
SOURCE: Chimie et Industrie (Paris) (1950), 63(No. 3 bis), 483-8
CODEN: CHIEAN; ISSN: 0009-4358
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Benzothiazole (I), benzoselenazole, and benzoxazole derivs. having in the 2-position a CH2COA group, where A is OEt, NHPh, NH2, NHNH2, or NHN:CHPh, condense readily with aromatic aldehydes, and heterocyclic alkylthio and 2-anilinovinyl cyclammonium salts to yield styryl, cyanine, and carbocyanine dyes. Et 2-benzothiazoleacetate (II) is prepared from EtO2CCH2COCl (III) and (o-H2NC6H4S)2Zn in C6H6 (cf. Staudinger and Becker, C.A. 12, 696). Similarly is prepared from (o-H2NC6H4Se)2Zn and III, Et 2-benzoselenazoleacetate, colorless crystals, m. 61-2°. Et 2-benzoxazoleacetate, m. 65-6°, is obtained from its Ag salt and EtI in CHCl3. II and PhNH2 in xylene in the presence of a trace of pyridine give 2-benzothiazoleacetanilide (IV), colorless crystals, m. 161-1.5°. II and concentrated aqueous NH3 yield 2-benzothiazoleacetamide, m. 175-6° (from EtOH). 2-Benzothiazoleacethydrazide (V), m. 151-2° (from EtOH), is prepared from II and H2NNH2.H2O in EtOH. V and BzH give benzaldehyde 2-benzothiazoleacethydrazone, m. 180-1° (from C5H11OH). Condensation of II and IV with p-Me2NC6H4CHO (VI) yields Et α-(4-dimethylaminobenzylidene)-2-benzothiazoleacetate (VII), m. 149-50°, λmaximum 400 mμ, log ε 4.54, and α-(4-dimethylaminobenzylidene)-2-benzothiazoleacetanilide (VIII), m. 223-4°, λmaximum 408 mμ, log ε 4.72, resp. Equimol. quantities of V and VI form a white precipitate, presumably p-dimethylaminobenzaldehyde 2-benzothiazoleacethydrazone (IX), which is converted by a 2nd mol. VI to the α-(4-dimethylaminobenzylidene) derivative (X) of IX, yellow solid, m. 211-12°, λmaximum 402 mμ, log ε 4.74. Condensation of I derivs. with 2-methylthiobenzothiazolium-MeX in EtOH in the presence of Et3N gives the following XI (A, m.p., λmaximum, and log ε given in the indicated order): OEt (XII), m. 148-9°, 385.5 mμ, 4.32; NHPh, m. 185-7°, 398.0 mμ, 4.52; NH2, m. 181-1.5°; and NHN: CHPh, m. 267-8°, 390 mμ, 4.69. From I derivs. and 2-(2-anilinovinyl)-1-ethylbenzothiazolium-MeX in EtOH in the presence of Ac2O are obtained the following carbocyanines XIII (A given): OEt (XIV), m. 162-2.5°; NHPh (XV), m. 172-4°; and NHN:CHPh (XVI), m. 185-7°. II heated with MeI in a sealed tube gives the methiodide, m. 170-1° (decompose) (from Me2CO), which gives with VI in Ac2O VII-MeI, m. 143-5°. Similarly are prepared XII-EtI, m. 187-8°; and XIV-EtI, m. 215-16°. Condensation of II with HC(OEt)3 in Ac2O yields by cyclization of the intermediate condensation product XVII, m. 294-5°; shows a strong blue fluorescence. The presence of the α-substituent of the type CH2COA in XIII shifts the absorption maximum (given) towards longer wave lengths as compared to the

L4 ANSWER 247 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
unsubstituted compd. (XVIII): XIV 489.1 mμ, log ε 4.80; XV 493.5 mμ, log ε 4.83; XVI 500.0 mμ, log ε 4.86; and XVIII 455.0 mμ, log ε 4.71. In XVIII-EtX 2 limiting structures of equal energy content having the pos. charge on either one of the 2 N make main contributions to the resonance hybrid, the introduction of an α-carbonyl substituent as in XIV-EtX causes the appearance of a 3rd electromeric form which destroys the energetic symmetry of the mol. and causes a hypsochromic effect lowering the absorption max. from 560 mμ (log ε 5.25) for XVIII-EtX to 504 mμ (log ε 4.82) for XIV-EtX. A similar bathochromic effect for the XI or a hypsochromic effect for XII-EtI as compared with the unsubstituted compds. (λmax. 388.5 mμ, log ε 4.82, and λmax. 424 mμ, log ε 4.65, resp.) is not observed because of steric hindrance preventing the coplanarity of the mol. and thus limiting the mesomeric forms of the mols. to 2 basic contributing structures. For similar reasons VII, VIII, and X do not show any bathochromic effect as compared with the unsubstituted compd. (λmax. 400 mμ, log ε 4.48). In VII-EtI the quaternization favors 2 contributing structures with either one of the 2 N bearing the pos. charge and causes a hypsochromic effect (λmax. 486 mμ) as compared with the unsubstituted analog (λmax. 524 mμ, log ε 4.60).
IT 875846-34-7, 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)- (derivs.)
RN 875846-34-7 CAPLUS
CN 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)- (5CI) (CA INDEX NAME)

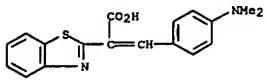


L4 ANSWER 248 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1952:26032 CAPLUS
DOCUMENT NUMBER: 46:26032
ORIGINAL REFERENCE NO.: 46:4402g-i,4403a-d
TITLE: Cyanine and styryl dyes
INVENTOR(S): van Dormael, Andre Emile; de Smet, Polydoor
PATENT ASSIGNEE(S): Gevaert Photo-Producten N. V.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

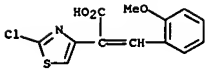
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 656515		19510822	GB 1947-8961	19470402

AB New monomethine cyanine and styryl dyes or their cyclammonium salts which are good photographic sensitizers or supersensitizers are prepared Thus 2-(benzoylmethyl)thiazole 2.4 g. is refluxed with p-Me2NC6H4CHO (I) 1.5 g. in AcOH 5 cc., for 2 hrs. Bright yellow crystals are obtained which give a supersensitizing effect with carbocyanine dyes. 5-Acetylmethyl-3-phenyl-1,2,4-oxadiazole and I give bright yellow crystals which supersensitize emulsions in the presence of a 2,2'-cyanine dye (Ia) with a maximum at 575-80 mμ. Et 2-benzothiazole-pyruvate and I give bright yellow crystals which super sensitize Ag emulsions in the presence of Ia with a maximum at 575-80 mμ. Et 2-benzothiazoleacetate (II) and I give bright yellow crystals which supersensitizes Ag emulsions over a broad range even beyond 600 mμ with a maximum at 460 and 570 mμ in presence of Ia, supersensitizes over a broad range to 620 mμ with a maximum at 560 mμ in presence of styryl dyes and shows a strong mutual supersensitizing effect to about 540 mμ in the presence of a compound prepared from 2-[2-(acetylanilino)vinyl]benzoxazole-EtI and p-(diethylamino)aniline sulfate in pyridine and m. 204-5°. II and 2-(methylmercapto)benzothiazole dimethyl sulfate (III) and Et3N give bright yellow crystals which supersensitize Ag emulsions in the presence of Ia with a maximum at 575 mμ. 2-Benzothiazoleacetanilide (IV) and I give bright yellow crystals which are supersensitizers in the presence of Ia with a maximum at 580 mμ. IV is prepared from II and aniline in the presence of pyridine; it m. 159-60°. Benzyl 2-benzothiazoleacetate (V) and I give crystals, m. 142-3°. In the presence of Ia it is a supersensitizer with a maximum at 580 mμ. V is a brownish oil which is prepared from o-aminothiophenol and benzyl cyanoacetate or ethyl benzyl malonate (VI). VI is prepared from K ethyl malonate and BzBr, it m. 197.0-9.5°. 2-Benzothiazoleacetamide (VII) and III give yellow crystals, m. 181.0-1.5°. It is a strong sensitizer for Ag emulsions up to 485 mμ. VII is prepared from ethyl 2-benzothiazoleacetate and NH4OH. Long, colorless needles are obtained, m. 171-2°. Ethyl 4-quinolineacetate and I give yellow needles, m. 135-6°. It is a strong supersensitizer for Ia with a maximum at 575 mμ. 2-(α-Phenylcarbamyl-p-dimethylaminostyryl)-benzothiazole and MeI give a dye, m. 178-80° (with decomposition). It is a supersensitizer for Ia. 2-Benzothiazolethioacetanilide (VIII) and I with piperidine give orange-yellow needles, m. 236.5-7.0°. It is a sensitizer of Ag emulsions up to 550 mμ with a broad maximum at 485 mμ. With Ia it has a maximum at 575 mμ. VIII is prepared from 2-benzothiazoleacetanilide and P2S5 in pyridine, it m. 168-72°.

L4 ANSWER 248 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Anisaldehyde and II with ZnCl2 give a dye m. 147-9°; it is a supersensitizer for Ia. Reaction of II and N,N'-pentamethylene-bis[2-(methylmercapto)benzothiazole bromide] with Et3N give a sensitizer, m. 148-50°, for Ag emulsions up to 485 mμ.
IT 875846-34-7, 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)-
(esters)
RN 875846-34-7 CAPLUS
CN 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)- (5CI) (CA INDEX NAME)

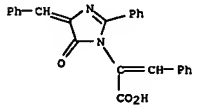


L4 ANSWER 249 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



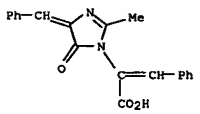
L4 ANSWER 249 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1950:52131 CAPLUS
DOCUMENT NUMBER: 44:52131
ORIGINAL REFERENCE NO.: 44:9960f-i,9961a-b
TITLE: Bromination of 3-acetocoumarin
AUTHOR(S): Koelsch, C. F.
CORPORATE SOURCE: Univ. of Minnesota, Minneapolis
SOURCE: Journal of the American Chemical Society (1950), 72, 2993-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Rap [Gazz. chim. ital. 27, II, 500 (1897)] reported that 3-acetylcoumarin (I) with Br yielded 3-acetyl-4-bromocoumarin; this compound is now shown to be 3-(bromoacetyl)coumarin (II). I (47 g.) in 200 ml. CHCl3, treated with 40 g. Br in 25 ml. CHCl3 (intermittent shaking and warming), and heated 15 min. on the water bath, gives 51-9 g. II, m. 163-5°. II (2.7 g.) in 15 ml. hot EtOH, with 1.6 g. CS(NH2)2 gives (after boiling with H2O containing AcONa) 2.2 g. 2-amino-4-(3-coumarinyl)thiazole (III), bright yellow, m. 225-7°. III (18 g.), 100 ml. AcOH, 200 ml. concentrated HCl, and 40 ml. BuNO2, mixed at 15° and kept 12 hrs. at room temperature, give 9.5 g. 2-chloro-4-(3-coumarinyl)thiazole (IV), m. 170-1°; 1 g. IV, warmed 10 min. with 5 ml. piperidine, gives 0.9 g. 4-(3-coumarinyl)-2-(1-piperidyl)thiazole, deep yellow, b15 310-15°, m. 132-3°; IV and PhNH2 give a gelatinous compound which with Ac2O yields 2-(N-acetylanilino)-4-(3-coumarinyl)thiazole, yellow, m. 230-1°. IV (4.7 g.) and 2.5 g. NaOH in 10 ml. EtOH and 25 ml. H2O, boiled 5 min. and treated with Me2SO4 and NaOH, give 3.2 g. α-(2-chloro-4-thiazolyl)-o-methoxycinnamic acid (V), pale yellow, m. 142-3°; 1.5 g. V and 0.3 g. Na2CO3 in 10 ml. H2O at 20°, treated with 70 ml. 4% KMnO4, give about 200 mg. o-MeOC6H4CHO and 400 mg. 2-chloro-4-thiazolecarboxylic acid, m. 220-1° (decomposition). II (2.7 g.) and 2 g. PhNH2 in 15 ml. EtOH, boiled 15 min., give 2.6 g. 3-(anilinoacetyl)coumarin, red, m. 180-5° (decomposition); Ac derivative, pale yellow, m. 181-2°. II (8 g.) in 100 ml. hot PhMe, treated with 2.5 g. C5H5N and kept 4 hrs. at room temperature, gives 9.7 g. 1-[2-(3-coumarinyl)-2-oxoethyl]pyridinium bromide (VI), pale yellow, decompose about 218°; NaOH gives a gelatinous precipitate which dries to scales resembling Fe(OH)3; the 2-Me derivative (VII) of VI, yellow brown, decompose about 200°; quinolinium analog of VI, orange-brown, decompose about 210°. 3-Carbethoxy-1-[2-(3-coumarinyl)-2-oxoethyl]pyridinium bromide, decompose about 190°; 4-carbethoxy isomer, decompose about 170°.
IT 859479-01-9P, 4-Thiazoleacetic acid, 2-chloro-α-o-methoxybenzylidene-
RL: PREP (Preparation)
(preparation of)
RN 859479-01-9 CAPLUS
CN 4-Thiazoleacetic acid, 2-chloro-α-o-methoxybenzylidene- (5CI) (CA INDEX NAME)

L4 ANSWER 250 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1944:8262 CAPLUS
DOCUMENT NUMBER: 38:8262
ORIGINAL REFERENCE NO.: 38:1210a-e
TITLE: Anhydrides of peptides and dehydrogenated peptides
AUTHOR(S): Tietzman, Josephine E.; Doherty, David G.; Bergmann, Max
SOURCE: Journal of Biological Chemistry (1943), 151, 387-94
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB By heating 20 g. of AcNHC(:CHPh)CONHC(:CHPh)CO2H (I) with 40 ml. of H2O and C5H5N for 4 hrs. at 90°, 8 g. of anhydro-I (II) m. 210-12°, was obtained. Reduction of II by H and Pd gave AcNHCH(CH2Ph)CONHCH(CH2Ph)CO2H, m. 245-6°, and a compound C20H2003N2, m. 199-200°, Me ester, 135-7°, probably O.CMe:N.CH(CH2Ph).C:NCH(CH2Ph)CO2H, an anhydro peptide. It is not affected by solution at room temperature for 24 hrs. in H2O, N HCl, or NaHCO3. An attempt to prepare an anhydro peptide from AcNHC(:CHPh)CONHCH2CO2H (II) by heating in vacuo at 180° (Graenacher, C. A. 21, 1813) gave only tar. The C5H5N-H2O procedure used above failed to convert either II or the Bz derivative to an anhydro peptide. In the reaction between BzH and NH2CH2CO2H, a compound C20H16N2O3 (III), m. 256° (decomposition), was isolated in addition to the azlactone and polymeric benzylidineglycine (Dakin, C. A. 23, 4205). With NH4OAc, III gave an NH4 salt, and is possibly O.CMe:N.C(:CHPh).C:NC(:CHPh)CO2H. The azlactone of BzNHC(:CHPh)CONHC(:CHPh)CO2H (IV) (C. A. 38, 64.1) on treatment with C5H5N-H2O gave anydro-IV, m. 258-9° (decomposition). The action of N NaOH on AcNHC(:CHPh)CONHC(:CHPh)C:N.C(:CHPh).C(:O).O at room temperature gave an anhydro peptide, probably NH.C(:CHPh).CO.N.C(:CHPh).C:N.C(:CHPh)C:O m. 289° (decomposition)
IT 855164-67-9P, Cinnamic acid, α-(4-benzylidene-4,5-dihydro-5-oxo-2-phenyl-1-imidazolyl)- 855164-69-1P, Cinnamic acid, α-(4-benzylidene-4,5-dihydro-2-methyl-5-oxo-1-imidazolyl)-
RL: PREP (Preparation)
(preparation of)
RN 855164-67-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

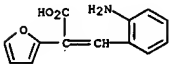


RN 855164-69-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

L4 ANSWER 250 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

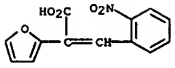


L4 ANSWER 251 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1943:14515 CAPLUS
DOCUMENT NUMBER: 37:14515
ORIGINAL REFERENCE NO.: 37:2371i,2372a-c
TITLE: Condensation of 2-furanacetic acid with o-nitrobenzaldehyde
AUTHOR(S): Amstutz, E. D.; Spitzmiller, Ervin R.
SOURCE: Journal of the American Chemical Society (1943), 65, 367-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB K 2-furanacetate (16.5 g.), added to 15.1 g. o-O2NC6H4CHO in 180 cc. Ac2O, the mixture heated at 75° for 12 h. (1 h. to temperature), the solution poured into 300 cc. H2O and neutralized with solid Na2CO3, 400 cc. H2O added, the solution filtered to free it from the insol. tarry substances and acidified, gives 26 g. of a dark green to yellow-brown product; dispersion in boiling H2O gives a solution of trans-α-2-furyl-o-nitrocinnamic acid (I), bright yellow, m. 137.6-8.2° (m. ps. corrected), and as a residue the cis-isomer (II), m. 192-2.4°; the yields were 23.2 and 42.6%. I (450 mg.) in 10 cc. PhNO2 and a crystal of iodine, heated at 210° for 40 min., gives 58% of II; after 20 min., the conversion was about 40%.
I heated with Cu chromite in quinoline gives 15% of trans-o-nitrophenyl-2-furylethylene (III), pale yellow, m. 92.8-3.6°; II (4 g.) gives 2 g. of the cis-isomer (IV), a light brown liquid, b3 152-4°, which did not crystallize. III heated in quinoline for 10 h. at 230° gives a small quantity of a light yellow compound, which was not identified as IV.
Reduction of I by FeSO4 in dilute NH4OH gives 78% of α-2-furyl-o-aminocinnamic acid (V), salmon-yellow, m. 156°; in sunlight it is changed to a tan-yellow. Attempted Pschorr ring closures on V were unsuccessful.
IT 855165-01-4P, Cinnamic acid, o-amino-α-2-furyl-
859999-37-4P, Cinnamic acid, α-2-furyl-o-nitro-, cis-
RL: PREP (Preparation)
(preparation of)
RN 855165-01-4 CAPLUS
CN Cinnamic acid, o-amino-α-2-furyl- (4CI) (CA INDEX NAME)



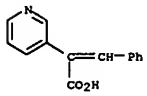
RN 859999-37-4 CAPLUS
CN 2-Furanacetic acid, α-(o-nitrobenzylidene)- (4CI) (CA INDEX NAME)

L4 ANSWER 251 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 252 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1942:33209 CAPLUS
DOCUMENT NUMBER: 36:33209
ORIGINAL REFERENCE NO.: 36:5175e-i
TITLE: 3-Pyridineacetic acid (β-homonicotinic acid)
AUTHOR(S): Hartmann, Max; Bosshard, Werner
SOURCE: Helvetica Chimica Acta (1941), 24, 28-35E
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 36:33209
AB A simple method for the production of the previously unknown 3-pyridineacetic acid (I) is described. 3-Pyridyl Me ketone (13 g.) in 100 cc. aqueous (NH4)2S and 10 g. S in 80 cc. dioxane were autoclaved for 6 hrs. at 160-70°. The reaction product was evaporated to dryness in vacuo. The residue was extracted with H2O and the extract was taken down to dryness. Crystallization from alc. by the addition of ether gave 3-pyridineacetamide (II), C7H8N2O, m. 123°. Refluxing 30 g. of crude residue with 300 cc. MeOH in the presence of HCl for 3 hrs. gave Me 3-pyridineacetate (III), b10 112°, hydrolyzed in 10% KOH in MeOH to I, C7H7NO2, m. 144°; Et ester, b12 124°; diethylamide, b12 175°.
III (7.65 g.) in 20 cc. absolute alc. and 20 cc. AcOH was catalytically reduced in the presence of 0.5 g. PtO2. Distillation of the product yielded an acetate (IV), b12 114°, dissociated by steam to Me 3-piperidineacetate, C10H19NO4, which, when recrystd. from a mixture of MeOH and acetone, in. 115-18°. A mixture of 1.0 g. IV in 1 cc. H2O, 0.5 g. of 85% HCO2H and 0.7 cc. of 40% HCHO was heated for 2 hrs. on the steam bath and then evaporated to dryness in vacuo. Esterification of the oily product gave 0.62 g. of Me 1-methyl-3-piperidineacetate, b13 96°, also produced by the catalytic reduction of the Me2SO4 compound of III, and yielding a picrate, m. 112-15°. The MeI derivative from 3.1 g. III was shaken with Ag2O (from 4 g. AgNO3) for 20 hrs. Working up gave the extremely hygroscopic 3-pyridineacetic acid methylbetaine, C8H9NO2, m. 130-2° (decomposition); HCl salt, m. 167° (decomposition); picrate, m. 154-6°. Boiling 10 g. III with 1.5 g. Na and 3.4 g. BzH in 30 cc. absolute ether for 20 hrs., treatment with 65 cc. N HCl and extraction with ether gave an oily ester, b0.2 157°, saponified to α-[3-pyridyl]cinnamic acid, C14H11NO2, m. 233° (decomposition) on recrystn. from alc.
IT 32967-19-4P, 3-Pyridineacetic acid, α-benzylidene-
RL: PREP (Preparation)
(preparation of)
RN 32967-19-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)

L4 ANSWER 252 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



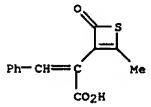
L4 ANSWER 253 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1939:54165 CAPLUS
DOCUMENT NUMBER: 33:54165
ORIGINAL REFERENCE NO.: 33:7779f-i
TITLE: Preparation of thiophene derivatives from ethyl β- carbethoxylevulinate
AUTHOR(S): Mitra, S.; Chakrabarty, N. K.; Mitra, S. K.
SOURCE: Journal of the Chemical Society (1939) 1116-17
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Ac(EtO2C)- CHCH2CO2Et, dissolved in an alc. previously saturated with HCl at 0° and treated with H2S for 12 hrs., gives the ethers of Et 5-hydroxy-2-methylthiophene-3-carboxylate: Me, b5 125°; Et, greenish yellow, b5 150°; Pr, yellow, b5 135°; refluxing with 10% Ba(OH)2 for 4-6 hrs. gives the free acids: 5-methoxy-2-methylthiophene-3-carboxylic acid (I), m. 128°; 5-EtO analog (II), m. 122° (Ba salt, needles); 5-PrO analog (III), m. 75°. II and BzH with EtOH-HCl (1 hr. at 0°) give di(5-ethoxy-3-carboxy-2-methylthienyl)phenylmethane (IV), m. 233°; vanillin gives the 4'-hydroxy-3'-methoxy derivative of IV, m. 235°; III and BzH give the PrO analog of IV, m. 232° (decomposition), and I gives the MeO analog, m. 250° (decomposition). I or II with HBr (mixed at 0° and allowed to stand at room temperature for 1 hr.) gives 5-hydroxy-2-methylthiophene-3- carboxylic acid (V), m. 160°; FeCl3 gives an intense pink color. V and BzH give with EtOH-HCl at room temperature for 1 hr. 5-keto-4-benzylidene-2-methyl-4,5-dihydrothioph.acte.ine-3- carboxylic acid, bright yellow, m. 166°; 4-o-nitrobenzylidene analog, bluish yellow, m. 184° (decomposition); 4- methoxybenzylidene analog, brilliant orange-yellow, m. 152°. V and AcH give the 4-ethylidene compound, hay- colored, m. 124°; cinnamaldehyde gives the 4-cinnamylidene compound, orange, m. 204°.

IT 858807-09-7P, Succinic acid, α-benzylidene-β-1-mercaptoethylidene-, thio lactone
RL: PREP (Preparation)
(preparation of)

RN 858807-09-7 CAPLUS
CN Succinic acid, α-benzylidene-β-1-mercaptoethylidene-, thio lactone (4CI) (CA INDEX NAME)



L4 ANSWER 254 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1935:1109 CAPLUS
DOCUMENT NUMBER: 29:1109
ORIGINAL REFERENCE NO.: 29:135h-i,136a-g
TITLE: Certain reactions of Γ-ketonic acids
AUTHOR(S): Allen, C. F. H.; Normington, J. B.; Wilson, C. V.
SOURCE: Can. J. Research (1934), 11, 382-94
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

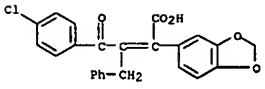
AB cf. C. A. 27, 2143. The following chalcones and derivs. are described: 2'-chloro-5'-methyl, b6 195-200°; dibromide, m. 117°; 2'-methyl-5'-isopropyl, b12 205-10°; dibromide, m. 140-1°; 3,4-methylenedioxy-4'-chloro, m. 128°; 4'-fluoro, m. 76-7°; 2',4',6'-tri-methylchalcone dibromide, m. 131°. 3,4-Methylenedioxy-benzoyl-p-chlorobenzoylmethane, m. 151°; benzoylmesitoyl-methane (mesitoyl = 2,4,6-Me3C6H2CO), m. 84°; 3-p-chlorobenzoyl-5-piperonylisoxazole, m. 180°; 3-mesityl-5-phenylisoxazole, m. 76°; α-bromobenzal-2,4,6-trimethylacetophenone, m. 73°. The following nitriles, corresponding acids and esters of the α-aryl-β-aroyl propionic acid series were prepared: α-phenyl-β-(4-fluorobenzoyl)-propionitrile, m. 102°; acid, m. 161°; Me ester, 101°; α-phenyl-β-(4-phenylbenzoyl)propionitrile, m. 176°; Me ester, m. 157°; α-phenyl-β-(p-toluyl)propionitrile, m. 80°; acid, m. 152°; Me ester, 112°; α-phenyl-β-(4-nitrobenzoyl)propionitrile, m. 155°; Me ester, m. 104°; α-phenyl-β-(4-carboxybenzoyl)propionitrile, m. 239°; di-Me ester, m. 110°; α-phenyl-β-(2-chloro-5-methylbenzoyl)propionitrile, m. 76-7°; Me ester, m. 80°; α-phenyl-β-mesitoylpropionitrile, m. 77-8°; acid, m. 172°; Me ester, m. 60-1°; α-piperonyl-β-(4-chlorobenzoyl)propionitrile, m. 129°; acid, m. 190°; Me ester, 109°; α-phenyl-β-(4-bromobenzoyl)propionic acid, m. 160°; Me α-piperonyl-β-benzoylpropionate, m. 121°; β-(4-chlorobenzoyl)propionic acid, m. 131°; Me ester, m. 63°; β-mesitoylpropionic acid, m. 107°. The following lactols (ketonic acids), derivs. of acrylic acid, are described: α-phenyl-β-benzyl-β-mesitoyl, m. 250° (decomposition); α-piperonyl-β-benzyl-β-(4-chlorobenzoyl), m. 153°; p-bromoanilide, m. 176°; α-piperonyl-β-benzyl-β-benzoyl, m. 138°; α-phenyl-β-benzyl-β-(4-phenylbenzoyl), m. 144°; chloride, m. 150°; α-phenyl-β-benzyl-β-(p-toluyl), m. 133°; α-phenyl-β-benzyl-β-(4-carboxybenzoyl), m. 240°; Me ester, m. 137°; chloride, m. 197°; α-phenyl-β-(2-chlorobenzyl)-β-(4-chlorobenzoyl), m. 147°; α-anisyl-β-(2-methoxybenzyl)-β-benzoyl, m. 126°; α-phenyl-β-(2-chlorobenzyl)-β-benzoyl, m. 98°; α-anisyl-β-(2-chlorobenzyl)-β-benzoyl, m. 154°; α-anisyl-β-(α-furylmethyl)-β-benzoyl, m. 121°. The highly substituted acrylic acids were treated with the Grignard reagent to differentiate between the 2 possible structures (lactol or open-chain acid). AcCl was found to be a satisfactory confirmatory reagent, giving chlorides with the lactols but not with the open-chain acids. From the available evidence it is concluded that the differences may be attributed to cis-trans isomerism. The α-aryl-β-aroyl propionic acids and the β-aroyl propionic acids were investigated with both reagents. The Grignard reagent

L4 ANSWER 254 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

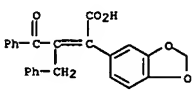
indicated mostly open-chain structures. The use of AcCl led to a variety of products; by varying the procedure, dimers of undetd. structure, unsaturated ketones, enolic acetates and Me esters were obtained. α-Phenyl-β-(p-chlorobenzoyl)propionic acid with AcCl gives C32H24O5Cl2, m. 235° (decompn.). α-Phenyl-β-mesitoylpropionic acid with AcCl yields a crotolactone, m. 126°, and a substance of high m. p. α-Phenyl-β-benzyl-β-(4-chlorobenzoyl)-propionic acid, m. 173-4°, is formed by the reduction of the corresponding acrylic acid. β-(p-Chlorobenzoyl)propionic acid and AcCl give Γ-(p-chlorophenylcrotolactone). Similarly β-mesitoylpropionic acid gives a compd., C26H24O4, (Pechmann dye?) and the enol-acetate. CH2.(CH2)4.C:O with AcCl gives the acetate. The mechanism of the reactions is discussed, as well as evidence for the possible structures of derivs. of Ac(CH2)2CO2H. A mechanism is suggested for the formation of enolic esters and unsatd. lactones of enolized ketonic acids. Numerous tables of results are included.

IT 857828-53-6P, Crotonic acid, β-p-chlorobenzoyl-α-(3,4-methylenedioxyphenyl)-γ-phenyl- 857828-67-2P, Crotonic acid, β-benzoyl-α-(3,4-methylenedioxyphenyl)-γ-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 857828-53-6 CAPLUS
CN Crotonic acid, β-p-chlorobenzoyl-α-(3,4-methylenedioxyphenyl)-γ-phenyl- (3CI). (CA INDEX NAME)



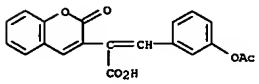
RN 857828-67-2 CAPLUS
CN Crotonic acid, β-benzoyl-α-(3,4-methylenedioxyphenyl)-γ-phenyl- (3CI) (CA INDEX NAME)



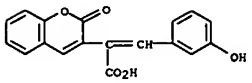
L4 ANSWER 255 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1934:50529 CAPLUS
DOCUMENT NUMBER: 28:50529
ORIGINAL REFERENCE NO.: 28:6131i,6132a-f
TITLE: Reactivity of the methylene group in coumarin-3-acetic acids. Condensation with aromatic aldehydes
AUTHOR(S): Dey, B. B.; Sankaranarayanan, Y.
SOURCE: J. Indian Chem. Soc. (1934), 11, 381-7
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C. A. 26, 3499. A comparison of the activities of the CH2 groups in PhCH2CO2H and coumarin-4-acetic acids has shown the latter to be more reactive. It may be argued that the activity of this group in coumarin-3-acetic acids is lower than that in the 4-acetic acids since, while the latter and their Et esters condensed easily with aldehydes under the conditions of both the Perkin and Knoevenagel reactions, coumarin-3-acetic acids (I) can only be made to react by Perkin's method. A mixture of the Na salt of I (3 g.), freshly distilled BzH (1.4 g.) and 12 g. of Ac2O was refluxed at 160° for 5 hrs. The product was decomposed by boiling in H2O and yielded 1.4 g. of phenyl-3-coumarylethylenecarboxylic acid, m. 202°. A similar condensation with p-HOC6H4CHO gave a solid product which dissolved in contact with dilute alkali, leaving a residue (II). Acidification of the solution gave p-acetoxyphenyl-3-coumarylethylenecarboxylic acid (III), m. 244°. Repeated recrystn. of II produced p-acetoxyphenyl-3-coumarylethylene (IV), m. 165°. Hydrolysis of III and IV by boiling with 2.0 N NaOH for 30 min. yielded the corresponding p-HO compds., m. 272° and 227°, resp. In contrast with the behavior of the 4-acetic acids which yielded only coumarinphenylethylenes by the Perkin reaction the condensation products from the 3-acetic acids consist mainly of the ethylenecarboxylic acids, existing chiefly in the form of the saturated lactones which are sufficiently stable to resist the action of Na2CO3 but which are converted by alkali into the salts of the free acids, from the solns. of which the original lactones are repptd. on acidification. The alternative view that the action of alkalies entails a fission of the pyrone and not of the new lactone ring is equally plausible. The following compds. were prepared by condensing coumarin-3-acetic acids with various aldehydes: 3-coumarylethylene-carboxylic acids; m-acetoxyphenyl (V), m. 188° (hydrolyzed to the m-HO compound, m. 242°); 3-methoxy-4'-acetoxyphenyl, m. 207° (hydrolyzed to 3'-methoxy-4'-hydroxyphenyl, m. 211°), 4'-methoxyphenyl, m. 225°, 3',4'-methylenedioxyphenyl, m. 270°, βα-naphtho-3-coumarylphenylethylenecarboxylic acid, m. 253°, 7-acetoxy-4-methyl-3-coumaryl-3'-coumarin, m. 268°, 7,7'-diacetoxy-4-methyl-3,3'-bicoumarin, m. 220°, 7-acetoxy-4-methyl-3-coumaryl-3'-βα-1,2-naphthopyrone, m. 272°, 3,3'-bi-βα-naphthopyrone, m. 345°, and the 3-coumarylethylenes, m-acetoxyphenyl, m. 140°, the by-product in the preparation of V, and its hydrolysis product m-hydroxylphenyl, m. 193°. The products of condensation of p-HOC6H4CHO and vanillin

L4 ANSWER 255 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto-, acetate (3CI) (CA INDEX NAME)



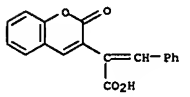
RN 876498-00-9 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto- (3CI) (CA INDEX NAME)



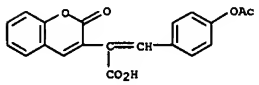
L4 ANSWER 255 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
with I exhibit the same color changes when treated with alkali as the analogous products derived from the 4-acetic acids. They are assumed to tautomerize readily, in the presence of alkalies, into quinonoid forms which, however, revert to the normal structure through opening of the pyrone ring by prolonged contact with alkali.

IT 860564-98-3P, 1,2-Benzopyran-3-acetic acid, α-benzal-2-keto-
872276-36-3P, 1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto-, acetate 876497-98-2P,
1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto-
876497-99-3P, 1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto-, acetate 876498-00-9P,
1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto-
RL: PREP (Preparation)
(preparation of)

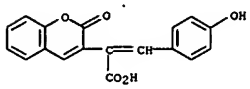
RN 860564-98-3 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-benzal-2-keto- (3CI) (CA INDEX NAME)



RN 872276-36-3 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto-, acetate (3CI) (CA INDEX NAME)



RN 876497-98-2 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto- (3CI) (CA INDEX NAME)



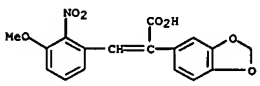
RN 876497-99-3 CAPLUS

L4 ANSWER 256 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1931:32742 CAPLUS
DOCUMENT NUMBER: 25:32742
ORIGINAL REFERENCE NO.: 25:3653g-i
TITLE: Synthesis of 4-methoxy-6,7-methylenedioxyphenanthrene and 4-methoxy-5,6-methylenedioxy-9-phenanthrenecarboxylic acid
AUTHOR(S): Girardet, A.
SOURCE: Helvetica Chimica Acta (1931), 14, 513-5
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The condensation of 18 g. of 3,4-(CH2O2)C6H3CH2CO2H (C. A. 18, 3385) with 18.1 g. of 2,3-O2N(MeO)-C6H3CHO (Ber. 28, 1385(1895)), in the presence of Ac2O and SnCl2 gave 18.5 g. of α-3,4-methylenedioxyphenyl-β-2-nitro-3-methoxyphenylacrylic acid, m. 225°. This was converted into the corresponding amino derivative, m. 221°, by the aid of NH3-FeSO4. By diazotization in 2 N H2SO4, boiling with mol. Cu and extraction of the cooled solution with Et2O, 4-methoxy-6,7-methylenedioxyphenanthrene-9-carboxylic acid, m. 271°, was formed. This acid was decarboxylated by sudden immersion in a metal bath at 300°, yielding a non-crystalline phenanthrene whose picrate, m. 160-1°, is not identical with that of the methylpukateine derivative By hydrolysis of 6-bromopiperonal azolactone with 10% NaOH and oxidation of the resulting pyruvic acid derivative, 5,6-(CH2O2)C6H3CH2CO2H, m. 192°, was prepared This was condensed with 2,3-O2N(MeO)C6H3CHO, the resulting product being reduced to the amino acid and converted by diazotization and consequent decomposition with mol. Cu into 4-methoxy-5,6-methylenedioxy-8-bromo-9-phenanthrenecarboxylic acid, m. 223°. This acid was debrominated by refluxing with alc. KOH and a Zn-Cu powder. Attempts to decarboxylate the non-brominated acid failed, some of the decomposition products esterifying the unchanged acid.

IT 860582-71-4P, Acrylic acid, α-(3,4-methylenedioxyphenyl)-β-2-nitro-m-anisyl-
RL: PREP (Preparation)
(preparation of)

RN 860582-71-4 CAPLUS
CN Acrylic acid, α-(3,4-methylenedioxyphenyl)-β-2-nitro-m-anisyl- (3CI) (CA INDEX NAME)



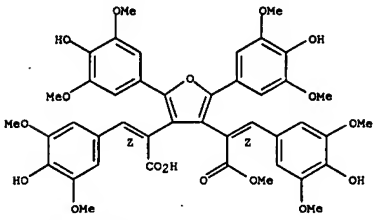
L4 ANSWER 1 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:21570 CAPLUS
DOCUMENT NUMBER: 146:287840
TITLE: Biotransformation of sinapic acid catalyzed by Momordica charantia peroxidase
AUTHOR(S): Liu, Hai-Li; Wan, Xiang; Huang, Xue-Feng; Kong, Ling-Yi
CORPORATE SOURCE: Department of Natural Medicinal Chemistry, China Pharmaceutical University, Nanjing, 210009, Peop. Rep. China
SOURCE: Journal of Agricultural and Food Chemistry (2007), 55(3), 1003-1008
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Biotransformation of sinapic acid with H2O2/Momordica charantia peroxidase, which exists in the widely used food M. charantia, at pH 5.0, 43°, in the presence of acetone resulted in six compds., including four new compds. (I-IV). Their structures were established on the basis of spectroscopic data. Compound IV showed a stronger antioxidative activity than the parent sinapic acid. Compds. III and IV significantly inhibited the growth of HL-60 cell at the concentration of 10-5 mol/L.
IT 927819-53-2P
RL: BPN (Biosynthetic preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(biotransformation of sinapic acid catalyzed by Momordica charantia peroxidase)
RN 927819-53-2 CAPLUS
CN 3-Furanacetic acid, 2,5-bis(4-hydroxy-3,5-dimethoxyphenyl)-4-[(12)-2-(4-hydroxy-3,5-dimethoxyphenyl)-1-(methoxycarbonyl)ethenyl]-α-[(4-hydroxy-3,5-dimethoxyphenyl)methylene]-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

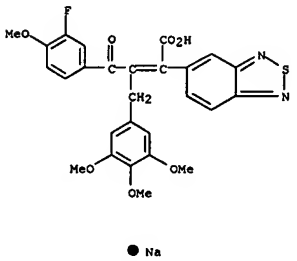
L4 ANSWER 1 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:828635 CAPLUS
DOCUMENT NUMBER: 145:207860
TITLE: Role of endothelin receptor activation in secondary pulmonary hypertension in awake swine after myocardial infarction
AUTHOR(S): Houweling, Birgit; Merkus, Daphne; Sorop, Oana; Boomsma, Frans; Duncker, Dirk J.
CORPORATE SOURCE: Experimental Cardiology, Thoraxcentre, Cardiovascular Research Institute COEUR, Erasmus MC, University Medical Centre Rotterdam, Rotterdam, Neth.
SOURCE: Journal of Physiology (Oxford, United Kingdom) (2006), 574(2), 615-626
CODEN: JPHYA7; ISSN: 0022-3751
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We previously observed that pulmonary hypertension secondary to myocardial infarction (MI) in swine is characterized by elevated plasma endothelin (ET) levels and pulmonary vascular resistance (PVR). Consequently, we tested the hypothesis that an increased ET-mediated vasoconstrictor influence contributes to secondary pulmonary hypertension after MI and investigated the involvement of ETA and ETB receptor subtypes. Chronically instrumented swine with (MI swine; n = 25) or without (normal swine; n = 19) MI were studied at rest and during treadmill exercise (up to 4 km h-1), in the absence and presence of the ETA antagonist EMD 122946 or the mixed ETA/ETB antagonist tezosentan. In normal swine, exercise caused a small decrease in PVR. ETA blockade had no effect on PVR at rest or during exercise. Conversely, ETA/ETB blockade decreased PVR but only during exercise (at 4 km h-1, from 3.0±0.1 to 2.3±0.1 mmHg min 1-1; P ≤ 0.05). MI increased pulmonary arterial pressure and PVR both at rest and during exercise (both P ≤ 0.05). The increased pulmonary arterial pressure correlated with the increased plasma ET levels in resting MI swine (r = 0.71; P ≤ 0.01). Furthermore, the pulmonary vasoconstrictor response to ET-1 infusion was enhanced after MI (P ≤ 0.05). ETA/ETB blockade decreased PVR in MI swine from 3.6±0.3 to 3.1±0.5 mmHg min 1-1 at rest and from 3.4±0.3 to 2.4±0.2 mmHg min 1-1 during exercise at 4 km h-1 (both P ≤ 0.05). This increased response to mixed ETA/ETB blockade in MI compared to normal swine appeared to be the result of an increased ETA-mediated vasoconstriction, as ETA blockade decreased PVR in MI swine from 3.4±0.4 to 2.8±0.2 mmHg min 1-1 at rest and from 3.1±0.3 to 2.6±0.2 mmHg min 1-1 at 4 km h-1 (both P ≤ 0.05). In conclusion, increased plasma ET levels together with increased pulmonary resistance vessel responsiveness to ET result in an exaggerated pulmonary vasoconstrictor influence of ET in swine with a recent MI. This vasoconstrictor influence is the result of an emergent tonic ETA-mediated vasoconstriction in addition to the exercise-induced ETB-mediated vasoconstriction that is already present in normal swine.
IT 195505-94-3, EMD122946
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect of endothelin receptors antagonist on secondary pulmonary hypertension)

L4 ANSWER 2 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 195505-94-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:513632 CAPLUS
DOCUMENT NUMBER: 145:23310
TITLE: Diagnostic use of endothelin ETB receptor agonists and
ETA receptor antagonists in tumor imaging
INVENTOR(S): Gulati, Anil; Gulati, Kartike
PATENT ASSIGNEE(S): The Board of Trustees of the University of Illinois, USA
SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006057988	A2	20060601	WO 2005-US42258	20051121
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

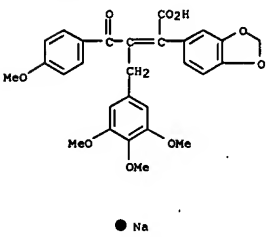
PRIORITY APPLN. INFO.: US 2004-629923P P 20041122

AB Methods of imaging tumors, such as breast tumors, are disclosed. The methods utilize an endothelin ETB receptor agonist or an endothelin ETA receptor antagonist, in combination with an imaging agent, to detect a tumor in mammals, including humans. Examples are provided on the effects of IRL-1620 and BQ-788 on tumor imaging and on tumor response to paclitaxel and doxorubicin.

IT 162412-70-6, Pd 156707 204326-22-7, Pd 164333
219993-82-5
RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(diagnostic use of endothelin ETB receptor agonists and ETA receptor antagonists in tumor imaging)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

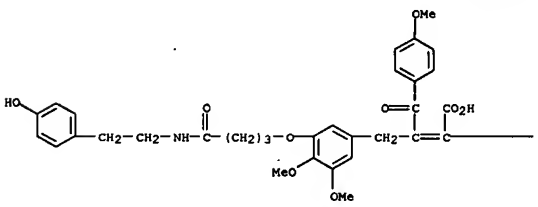
L4 ANSWER 3 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

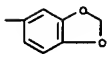
RN 204326-22-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-[4-[[2-(4-hydroxyphenyl)ethyl]amino]-4-oxobutoxy]-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

PAGE 1-A

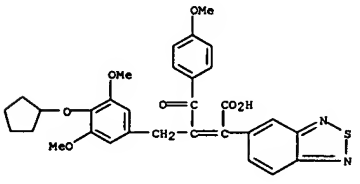


L4 ANSWER 3 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B



RN 219993-82-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:213386 CAPLUS
DOCUMENT NUMBER: 144:286183
TITLE: Endothelin a receptor (eta) antagonists in combination
with phosphodiesterase 5 inhibitors (pde5) and uses thereof
INVENTOR(S): Keyser, Donald Jeffrey; Dixon, Richard
PATENT ASSIGNEE(S): Encysive Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006026395	A1	20060309	WO 2005-US30342	20050826
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2006205733	A1	20060914	US 2005-211099	20050825
AU 2005280077	A1	20060309	AU 2005-280077	20050826

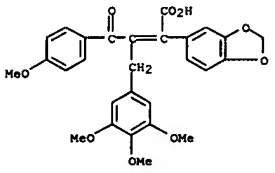
PRIORITY APPLN. INFO.: US 2004-604462P P 20040826
US 2005-211099 A 20050825
WO 2005-US30342 W 20050826

AB The invention relates generally to combination therapies comprising an endothelin A receptor (ETA) antagonist and a phosphodiesterase 5 (PDE5) inhibitor, pharmaceutical compns. comprising ETA antagonist and PDE5 inhibitor and methods of treating various disorders comprising administering an ETA antagonist and a PDE5 inhibitor. In particular, the combination therapies and pharmaceutical compns. are useful for the treatment and/or prevention of cardiac disorders such as pulmonary arterial hypertension (PAH). No significant pharmacokinetic interactions between sitaxsentan and sildenafil were demonstrated in healthy volunteers.

IT 162412-70-6, PD-156707 162412-71-7, PD-155080
195505-94-3, EMD-122946
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ETA antagonist and PDE5 inhibitor combinations for treating vascular disorders)

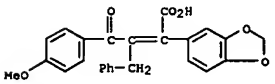
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

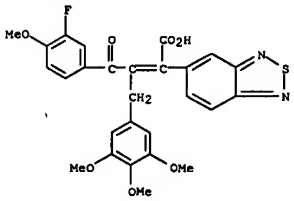
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

RN 195505-94-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:149262 CAPLUS
DOCUMENT NUMBER: 144:239931
TITLE: Pharmaceutical compositions for the treatment of respiratory and gastrointestinal disorders
INVENTOR(S): Jung, Birgit; Himmelsbach, Frank
PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany; Boehringer Ingelheim Pharma Gmbh & Co. KG
SOURCE: PCT Int. Appl., 321 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006015775	A2	20060216	WO 2005-EP8385	20050803
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2006035893	A1	20060216	US 2005-189643	20050726
CA 2575541	A1	20060216	CA 2005-2575541	20050803
PRIORITY APPLN. INFO.:			EP 2004-18808	A 20040807
			WO 2005-EP8385	W 20050803

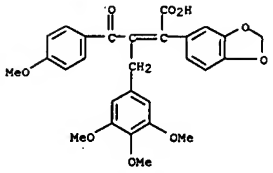
OTHER SOURCE(S): MARPAT 144:239931

AB The present invention relates to novel pharmaceutical compns. comprising at least 1 EGFR kinase inhibitor and at least one addnl. active compound selected from β-2 mimetics, steroids, PDE-IV inhibitors, p38 MAP kinase inhibitors, NK1 antagonists and endothelin-antagonists, processes for preparing the compns. and the use thereof as drugs in the treatment of respiratory or gastrointestinal complaints, as well as inflammatory diseases of the joints, the skin or the eyes. Thus, an inhalable powder contained an EGFR kinase inhibitor 150, formoterol fumarate dihydrate 50, and lactose 12,300 mg/capsule.

IT 162412-70-6
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmaceutical compns. for treatment of respiratory and gastrointestinal disorders)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

L4 ANSWER 6 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:735096 CAPLUS
DOCUMENT NUMBER: 143:199988
TITLE: Use of endothelin antagonists to prevent restenosis
INVENTOR(S): Carlyle, Wenda
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 16 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

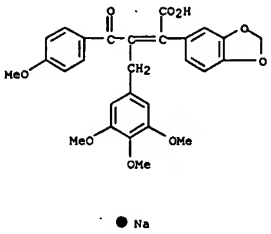
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005175667	A1	20050811	US 2005-54009	20050208
WO 2005077347	A1	20050825	WO 2005-US4315	20050210

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

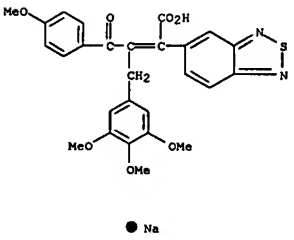
PRIORITY APPLN. INFO.: US 2004-543252P P 20040210
US 2005-54009 A 20050208

AB Provided are devices and methods for treating or preventing smooth muscle cell proliferation caused by endothelin-mediated conditions. In particular, a medical device comprising a structure which is implantable within a body lumen and means on or within the structure for releasing an endothelin (A) receptor antagonist at a rate effective to inhibit smooth muscle cell proliferation. The device can be, for example, an expansible stent or a graft, and the means can include a matrix coating, wherein the endothelin (A) receptor antagonist can be dispersed within the coating or disposed directly on the structure and under the matrix. The methods and devices of this invention can be used to decrease the incidence of restenosis as well as other thromboembolic complications resulting from implantation of medical devices. For example, Nitinol stents were cleaned in an ultrasonic bath with iso-Pr alc., dried and plasma cleaned in a plasma chamber. The cleaned stents were dip coated with an ethylene-vinyl alc. copolymer (EVOH) solution containing DMSO and Ambrisentan, and then passed over a hot plate, for about 3-5 s, with a temperature setting of about 60°. The coated stents were heated for 6 h in an air box and then placed in an oven at 60° under vacuum condition for 24 h to complete evaporation of the solvent.
IT 162412-70-6, PD-156707 195505-82-9, EMD-122801
RL: DEV (Device component use); THU (Therapeutic use); BIOL (Biological

L4 ANSWER 6 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study); USES (Uses)
(implantable devices comprising endothelin receptor antagonists for prevention of vascular smooth muscle cell proliferation)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



RN 195505-82-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:586215 CAPLUS
DOCUMENT NUMBER: 143:120526
TITLE: Pharmaceutical compositions based on anticholinergics and additional active ingredients
INVENTOR(S): Pairet, Michel; Pieper, Michael P.; Meade, Christopher
John Montague; Reichl, Richard; Schmelzer, Christel; Jung, Birgit
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. Kg, Germany
SOURCE: U.S. Pat. Appl. Publ., 50 pp., Cont.-in-part of U.S. Ser. No. 624,391.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148562	A1	20050707	US 2004-6940	20041208
DE 10062712	A1	20020620	DE 2000-10062712	20001215
DE 10063957	A1	20020627	DE 2000-10063957	20001220
DE 10110772	A1	20020912	DE 2001-10110772	20010307
DE 10111058	A1	20020912	DE 2001-10111058	20010308
DE 10113366	A1	20020926	DE 2001-10113366	20010320
DE 10138272	A1	20030227	DE 2001-10138272	20010810
US 2002151541	A1	20021017	US 2001-7182	20011019
US 2002183292	A1	20021205	US 2001-86145	20011019
US 2002137764	A1	20020926	US 2001-40196	20011025
US 2002122773	A1	20020905	US 2001-27662	20011220
DE 10206505	A1	20030828	DE 2002-10206505	20020216
US 2002169181	A1	20021114	US 2002-92116	20020306
US 6620438	B2	20030916		
US 2002193393	A1	20021219	US 2002-93240	20020307
US 2002183347	A1	20021205	US 2002-100659	20020318
US 6608054	B2	20030819		
US 2003158196	A1	20030821	US 2003-360064	20030207
US 2003181478	A1	20030925	US 2003-395777	20030324
US 6890517	B2	20050510		
US 2003203925	A1	20031030	US 2003-413065	20030414
US 2003212075	A1	20031113	US 2003-419358	20030421
US 6696042	B2	20040224		
US 2004024007	A1	20040205	US 2003-613783	20030703
US 2004151770	A1	20040805	US 2004-763894	20040123
US 2004161386	A1	20040819	US 2004-775901	20040210
US 2004176338	A1	20040909	US 2004-776757	20040211
US 2004192675	A1	20040930	US 2004-824391	20040414
US 2005147564	A1	20050707	US 2005-68134	20050228

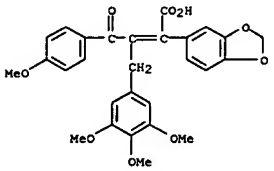
PRIORITY APPLN. INFO.: DE 2000-10054042 A 20001031
US 2000-253613P P 20001128
DE 2000-10062712 A 20001215
DE 2000-10063957 A 20001220
US 2000-257220P P 20001221
US 2000-257221P P 20001221

L4 ANSWER 7 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

DE 2001-10110772	A	20010307
DE 2001-10111058	A	20010308
DE 2001-10113366	A	20010320
US 2001-281653P	P	20010405
US 2001-281857P	P	20010405
US 2001-281874P	P	20010405
DE 2001-10138272	A	20010810
US 2001-314599P	P	20010824
US 2001-7182	B1	20011019
US 2001-86145	B1	20011019
US 2001-27662	B1	20011220
DE 2002-10206505	A	20020216
US 2002-92116	A1	20020306
US 2002-93240	B1	20020307
US 2002-100659	A1	20020318
US 2002-369213P	P	20020401
US 2003-360064	A2	20030207
US 2003-413065	B2	20030414
US 2003-419358	A1	20030421
US 2003-613783	A2	20030703
US 2004-763894	A2	20040123
US 2004-775901	A2	20040210
US 2004-776757	A2	20040211
US 2004-824391	A2	20040414
US 2001-40196	B1	20011025
US 2003-395777	A1	20030324

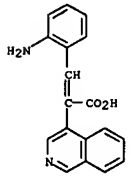
OTHER SOURCE(S): MARPAT 143:120526
AB A pharmaceutical composition comprising an anticholinergic and at least one addnl. active ingredient selected from among corticosteroids, dopamine agonists, PDE-IV inhibitors, NK1-antagonists, endothelin antagonists, antihistamines, and EGFR-kinase inhibitors, processes for preparing them and

L4 ANSWER 7 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
their use in the treatment of respiratory diseases. Among a no. of compds. prepd. was N-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-2-[4-[(3-hydroxypropyl)methylamino]piperidin-1-yl]-N-methyl-2-phenylacetamide. Inhalable powders include a formulation contg. tiotropium bromide, budesonide, and lactose.
IT 162412-70-6, Pd-156707
RL: MOA (Modifier or additive use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. based on anticholinergics and addnl. active ingredients)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

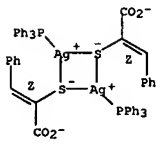
L4 ANSWER 8 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:409854 CAPLUS
Correction of: 2005:155226
DOCUMENT NUMBER: 143:248216
Correction of: 142:197775
TITLE: Product class 11: phenanthridines
AUTHOR(S): Keller, P. A.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2005), 15, 1065-1088
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of synthetic methods to prepare phenanthridines including cyclization, ring transformation, aromatization and substituent modification. The review includes phenanthridine 5-oxides and phenanthridinium salts.
IT 862586-45-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenanthridines, phenanthridine-5-oxides and phenanthridinium salts via cyclization, ring transformation, aromatization and substituent modification)
RN 862586-45-6 CAPLUS
CN 4-Isoquinolineacetic acid, α-[(2-aminophenyl)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:356330 CAPLUS
DOCUMENT NUMBER: 143:70419
TITLE: New structural features in triphenylphosphinesilver(I) sulfanylcarboxylates
AUTHOR(S): Barreiro, Elena; Casas, Jose S.; Couce, Maria D.; Sanchez, Agustin; Sordo, Jose; Varela, Jose M.; Vazquez-Lopez, Ezequiel M.
CORPORATE SOURCE: Departamento de Quimica Inorganica, Facultade de Farmacia, Universidade de Santiago de Compostela, Santiago de Compostela, Galicia, 15782, Spain
SOURCE: Dalton Transactions (2005), (9), 1707-1715
CODEN: DTARAF; ISSN: 1477-9226
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:70419
AB The authors studied the reactions of 1.5:1:1 mol ratio mixts. of PPh3, AgNO3 and 3-(aryl)-2-sulfanylpropenoic acids H2xspa in CHCl3/H2O, where spa = 2-sulfanylpropenoato and x = Ph (p), 2-ClC6H4 (Clp), 2-MeOC6H4 (o-mp), 4-MeOC6H4 (p-mp), 2-HO-3,5-Br2C6H2 (diBr-o-hp) or 2-furyl (f). Complexes [Ag(PPh3)(Hpspa)]2 (1), [(AgPPh3)2(xspa)]2 [x = Clp (2), o-mp (3), p-mp (4), diBr-o-hp (5) and f (6)] and [Ag(PPh3)3(Hfspa)] (7) were isolated, and all except 7 were characterized by IR, Raman and FAB mass spectrometry and by 1H, 13C and 31P NMR spectroscopy. Compound 6 was also characterized by 13C CP/MAS, and compds. 1 and 6 by 109Ag NMR spectroscopy. The crystal structures of 1, 2, 3, 4·Me2CO, 5, 6·Me2CO and 7 were determined by x-ray diffraction. Dimeric 1 has a supramol. structure based on H bonding between dinuclear units, and all the other complexes adopt discrete structures. 2, 3, 4·Me2CO, 5, and 6·Me2CO are tetranuclear, and 7 is mononuclear. The tetranuclear complexes contain the eight-membered coordination ring Ag4S2O2 (2, 3, 4·Me2CO, 6·Me2CO) or the twelve-membered ring Ag4(CO2)2S2 (5).
IT 854505-54-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR in solution)
RN 854505-54-7 CAPLUS
CN Argentate(2-), bis[μ-[(2Z)-2-(mercapto-κS:κS)-3-phenyl-2-propenoato(2-)]]bis(triphenylphosphine)di-, dihydrogen (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 9 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



●2 H+

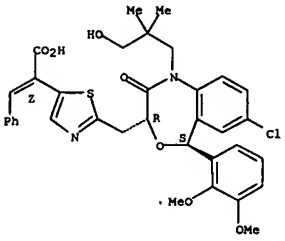
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:120907 CAPLUS
DOCUMENT NUMBER: 142:219318
TITLE: Preparation of benzoxazepine derivatives as squalene synthase inhibitors
INVENTOR(S): Marui, Shogo; Miki, Takashi; Miura, Shoutarou; Nishimoto, Tomoyuki; Nakada, Yoshihisa
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 239 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012272	A1	20050210	WO 2004-JP11293	20040730
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004260757	A1	20050210	AU 2004-260757	20040730
CA 2534464	A1	20050210	CA 2004-2534464	20040730
JP 2005068138	A	20050317	JP 2004-222658	20040730
EP 1650201	A1	20060426	EP 2004-748264	20040730
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1832934	A	20060913	CN 2004-80022202	20040730
BR 2004013009	A	20061003	BR 2004-13009	20040730
NO 2006001009	A	20060502	NO 2006-1009	20060301
PRIORITY APPLN. INFO.:			JP 2003-285341 A	20030801
			WO 2004-JP11293 W	20040730

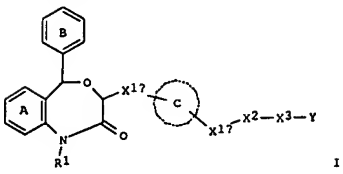
OTHER SOURCE(S): MARPAT 142:219318
GI

L4 ANSWER 10 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



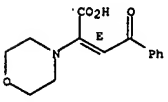
I

AB The title compds. I (ring A and ring B each represents an optionally substituted benzene ring; ring C represents an optionally further substituted aromatic ring; R1 represents a lower alkyl optionally substituted by optionally substituted hydroxy; X1a represents a bond or optionally substituted lower alkylene; X1b represents a bond or optionally substituted lower alkylene; X2 represents a bond, O, or S; X3 represents a bond or an optionally substituted divalent hydrocarbon group; and Y represents optionally esterified or amidated carboxy) are prepared A process for preparing I is disclosed. Thus, (2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepin-3-yl]methyl]-1,3-thiazol-5-yl)acetic acid was prepared in a multistep process from 2-(tert-butoxycarbonylamino)acetic acid and potassium monoethyl malonate. Compds. of this invention are said to show IC50 values of ≤ 1 μM against squalene synthase. Formulations are given.
IT 839724-03-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxazepine derivs. as squalene synthase inhibitors)
RN 839724-03-7 CAPLUS
CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

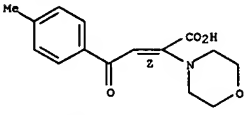
L4 ANSWER 11 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1008787 CAPLUS
DOCUMENT NUMBER: 142:392352
TITLE: Synthesis, antimicrobial, and analgesic activity of 4-aryl-2-N-morpholino-4-oxo-2-butenoic acids
AUTHOR(S): Koz'minykh, V. O.; Belyaev, A. O.; Koz'minykh, E. N.; Makhmudov, R. R.; Odegova, T. F.
CORPORATE SOURCE: Perm State Pharmaceutical Academy, Perm, Russia
SOURCE: Pharmaceutical Chemistry Journal (Translation of Khimiko-Farmatsevticheskii Zhurnal) (2004), 38(8), 431-433
CODEN: PCJOAU; ISSN: 0091-150X
PUBLISHER: Springer Science+Business Media, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:392352
AB The title compds. were prepared by treating the hydroxy analogs with morpholine. They have considerable analgesic activity, but are devoid of antibacterial activity.
IT 850143-07-6P 850143-08-7P 850143-09-8P 850143-10-1P 850143-11-2P 850143-12-3P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, antimicrobial, and analgesic activity of 4-aryl-2-N-morpholino-4-oxo-2-butenoic acids)
RN 850143-07-6 CAPLUS
CN 4-Morpholineacetic acid, α-(2-oxo-2-phenylethylidene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 850143-08-7 CAPLUS
CN 4-Morpholineacetic acid, α-[2-(4-methylphenyl)-2-oxoethylidene]-, (αZ)- (9CI) (CA INDEX NAME)

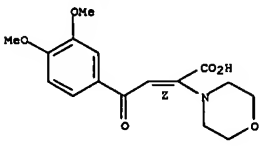
Double bond geometry as shown.



RN 850143-09-8 CAPLUS
CN 4-Morpholineacetic acid, α-[2-(3,4-dimethoxyphenyl)-2-oxoethylidene]-, (αZ)- (9CI) (CA INDEX NAME)

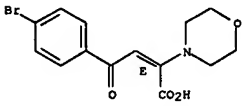
L4 ANSWER 11 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



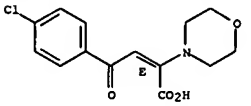
RN 850143-10-1 CAPLUS
CN 4-Morpholineacetic acid, α-[2-(4-bromophenyl)-2-oxoethylidene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 850143-11-2 CAPLUS
CN 4-Morpholineacetic acid, α-[2-(4-chlorophenyl)-2-oxoethylidene]-, (αE)- (9CI) (CA INDEX NAME)

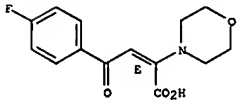
Double bond geometry as shown.



RN 850143-12-3 CAPLUS
CN 4-Morpholineacetic acid, α-[2-(4-fluorophenyl)-2-oxoethylidene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 11 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

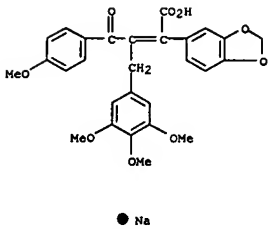
ACCESSION NUMBER: 2004:874884 CAPLUS
DOCUMENT NUMBER: 142:48477
TITLE: Use of Classification Regression Tree in Predicting Oral Absorption in Humans
AUTHOR(S): Bai, Jane P. F.; Utis, Andrey; Crippen, Gordon; He, Han-Dan; Fischer, Volker; Tullman, Robert; Yin, He-Qun; Hsu, Cheng-Pang; Jiang, Lan; Hwang, Kin-Kai
CORPORATE SOURCE: ZyxBio LLC, Hudson, OH, 44236, USA
SOURCE: Journal of Chemical Information and Computer Sciences (2004), 44(6), 2061-2069
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The purpose of this study is to explore the use of classification regression trees (CART) in predicting, in the dose-independent range, the fraction dose absorbed in humans. Since the results from clin. formulations in humans were used for training the model, a hypothetical state of drug mols. already dissolved in the intestinal fluid was adopted. Therefore, the mol. attributes affecting dissoln. were not considered in the model. As a result, the model projects the highest achievable fraction dose absorbed, providing a reference point for manipulating the formulations or solid states to optimize oral clin. efficacy. A set of approx. 1260 structures and their human oral pharmacokinetic data, including bioavailability and/or absorption and/or radio-labeled studies, were used, with 899 compds. as the training set and 362 the test set. The numerical range of the fraction dose absorbed, 0 to 1, was divided into 6 classes with each class having a size of approx. 0.16. A set of 28 structural descriptors was used for modeling oral absorption without considering active transport. Then, a sep. branch was created for modeling oral absorption involving active transport. The AAE of the training set was 0.12 and those of five test sets ranged from 0.17 to 0.2. In terms of classification, two test sets of unpublished, proprietary compds. showed 79% to 86% prediction when the predicted values fallen within ± one class of real values were considered predicted. Overall, the computational errors from all the test sets of diverse structures were similar and reasonably acceptable. As compared to artificial membranes for ranking drug absorption potential, prediction by the CART model is considered fast and reasonably accurate for accelerating drug discovery. One can not only improve continuously the accuracy of CART computations by expanding the chemical space of the training set but also calculate the statistical errors associated with individual decision paths resulting from the training set to determine whether to accept individual computations of any test sets.

IT 162412-70-6, PD 156707
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(use of classification regression tree in predicting oral absorption in humans)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA NAME)

L4 ANSWER 12 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

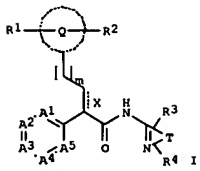
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

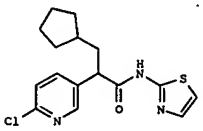
L4 ANSWER 13 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:696370 CAPLUS
DOCUMENT NUMBER: 141:225497
TITLE: Preparation of tri(cyclo) substituted amide glucokinase activator compounds
INVENTOR(S): Fyfe, Matthew Colin Thor; Gardner, Lisa Sarah; Nawano, Masao; Procter, Martin James; Williams, Geoffrey Martyn; Witter, David; Yasuda, Kosuke; Rasamison, Chrystelle Marie; Castelhano, Arlindo
PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004072066	A1	20040826	WO 2004-US3982	20040210
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004186290	A1	20040923	US 2004-776559	20040210
EP 1594863	A1	20051116	EP 2004-709897	20040210
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.:			
	US 2003-446682P	P	20030211
	US 2003-512826P	P	20030811
	WO 2004-US3982	W	20040210

OTHER SOURCE(S): MARPAT 141:225497
GI


I


II

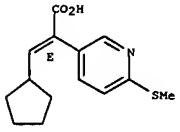
L4 ANSWER 13 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB The title compds. [I; one of A1-A5 = N, another = CR5, another = CR6, and the other two = N, CH; Q = cycloalkyl, 5-6 membered heteroaryl, 4-8 membered heterocyclyl; T together with N:C to which it is attached forms a heteroaryl or heteroacyclyl where the N:C bond is the only site of unsatn.; R1, R2 = H, halo, OH, CN, etc.; or R1 and R2 may be taken together to represent an oxygen atom attached to the ring via a double bond; R3, R4 = H, halo, CN, NO2, etc.; R5, R6 = H, OH, halo, CN, etc.; or R5 and R6 together form a 5-8 membered carbocyclic or heterocyclic ring; m = 0-1; X indicates that the double bond has the (E)-configuration; one proviso given] which are useful in the prophylactic and therapeutic treatment of hyperglycemia and diabetes, were prepared Thus, amidation of 2-(6-chloropyridin-3-yl)-3-cyclopentylpropionic acid (preparation given) with thiazol-2-ylamine afforded II. The exemplified compds. I produced EC50's ranging from 0.1 to 23.0 μM with max FAs from 1.7 to 6.7 in in vitro assay for GK activity. The pharmaceutical composition comprising the compound I is claimed.

IT 745816-32-4P 745816-34-6P 745816-35-7P
745816-36-8P 745816-37-9P 745816-38-0P
745816-39-1P 745816-42-6P 745816-45-9P
745816-46-0P 745816-51-7P 745816-59-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tricyclo substituted propionamides and acrylamides as glucokinase activators for treating hyperglycemia and diabetes)

RN 745816-32-4 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-(methylthio)-, (αE)- (9CI) (CA INDEX NAME)

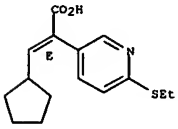
Double bond geometry as shown.



RN 745816-34-6 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-(ethylthio)-, (αE)- (9CI) (CA INDEX NAME)

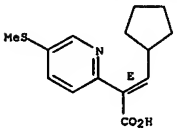
Double bond geometry as shown.

L4 ANSWER 13 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



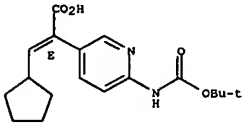
RN 745816-35-7 CAPLUS
CN 2-Pyridineacetic acid, α-(cyclopentylmethylene)-5-(methylthio)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 745816-36-8 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-[[(1,1-dimethylethoxy)carbonyl]amino]-, (αE)- (9CI) (CA INDEX NAME)

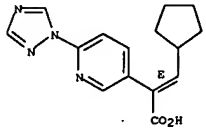
Double bond geometry as shown.



RN 745816-37-9 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-(1H-1,2,4-triazol-1-yl)-, (αE)- (9CI) (CA INDEX NAME)

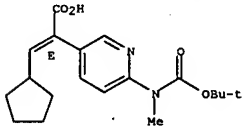
Double bond geometry as shown.

L4 ANSWER 13 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



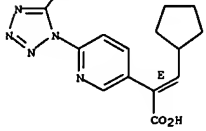
RN 745816-38-0 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-[[(1,1-dimethylethoxy)carbonyl]methylamino]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 745816-39-1 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-(5-methyl-1H-tetrazol-1-yl)-, (αE)- (9CI) (CA INDEX NAME)

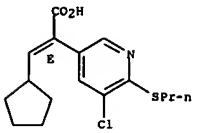
Double bond geometry as shown.



RN 745816-42-6 CAPLUS
CN 3-Pyridineacetic acid, 5-chloro-α-(cyclopentylmethylene)-6-(propylthio)-, (αE)- (9CI) (CA INDEX NAME)

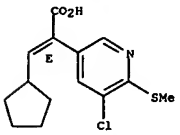
Double bond geometry as shown.

L4 ANSWER 13 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



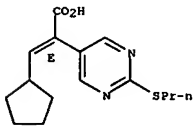
RN 745816-45-9 CAPLUS
CN 3-Pyridineacetic acid, 5-chloro-α-(cyclopentylmethylene)-6-(methylthio)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 745816-46-0 CAPLUS
CN 5-Pyrimidineacetic acid, α-(cyclopentylmethylene)-2-(propylthio)-, (αE)- (9CI) (CA INDEX NAME)

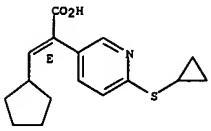
Double bond geometry as shown.



RN 745816-51-7 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-(cyclopropylthio)-, (αE)- (9CI) (CA INDEX NAME)

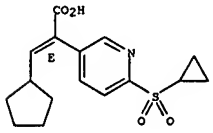
Double bond geometry as shown.

L4 ANSWER 13 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 745816-59-5 CAPLUS
CN 3-Pyridineacetic acid, α-(cyclopentylmethylene)-6-(cyclopropylsulfonyl)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

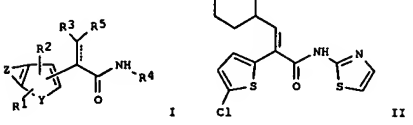


L4 ANSWER 14 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:606468 CAPLUS
DOCUMENT NUMBER: 141:140431
TITLE: Preparation of heteroaryl compounds for the treatment of type II diabetes
INVENTOR(S): Weichert, Andreas Gerhard; Barrett, David Gene; Heuser, Stefan; Riedl, Rainer; Tebbe, Mark Joseph; Zaliani, Andrea
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004063194	A1	20040729	WO 2003-US37089	20031216
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003294376	A1	20040810	AU 2003-294376	20031216
PRIORITY APPLN. INFO.:			US 2003-438538P P	20030106
			WO 2003-US37089 W	20031216

OTHER SOURCE(S): MARPAT 141:140431
GI



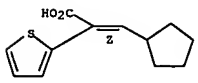
I II

AB Heteroaryl compds. of formula I [R1, R2 = H, halo, amino, nitro, CN, sulfonamido, alkyl, alkoxy, etc.; R3 = alkyl, arylalkyl, heterocycloalkyl, etc.; R4 = heteroarom., (substituted) CONH2, etc.; R5 = H, halo, alkyl; Y = O, S; Z = absent, CH=CH-CH=CH] are prepared These compds. are considered to be useful for the treatment of type II diabetes. Thus, II was prepd. from 5-chlorothiophen-2-ylboronic acid, (Z)-Et 3-cyclohexyl-2-iodopropenoate and 2-aminothiazole. II had ED50 of 1.840 μM for glucokinase activation.

L4 ANSWER 14 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 727695-39-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thiazolyl acetamides for treatment of type II diabetes)
RN 727695-39-8 CAPLUS
CN 2-Thiopheneacetic acid, α-(cyclopentylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

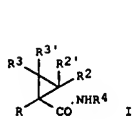


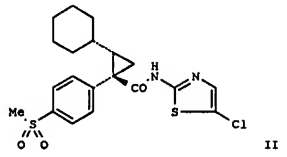
L4 ANSWER 15 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:606457 CAPLUS
DOCUMENT NUMBER: 141:157108
TITLE: Preparation of aryl substituted cyclopropylcarboxamides for therapeutic use as glucokinase activators
INVENTOR(S): Weichert, Andreas Gerhard; Barrett, David Gene; Heuser, Stefan; Riedl, Rainer; Tebbe, Mark Joseph; Zaliani, Andrea
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 141 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004063179	A1	20040729	WO 2003-US37088	20031216
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2509086	A1	20040729	CA 2003-2509086	20031216
AU 2003297291	A1	20040810	AU 2003-297291	20031216
EP 1585739	A1	20051019	EP 2003-815189	20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, BG, CZ, EE, HU, SK				
JP 2006515858	T	20060608	JP 2004-566494	20031216
US 2006111353	A1	20060525	US 2005-541047	20050629
PRIORITY APPLN. INFO.:			US 2003-438539P P	20030106
			WO 2003-US37088 W	20031216

OTHER SOURCE(S): MARPAT 141:157108
GI

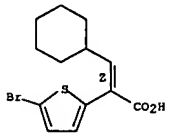
L4 ANSWER 15 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)


I


II

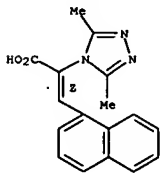
AB Cyclopropylcarboxamides, such as I [R = substituted aryl or heteroaryl; R2, R2' = H, Me, halogen; R3 = alkyl, cycloalkyl, cycloalkylmethyl, etc.; R3' = H, halogen, alkyl, perfluoroalkyl; R4 = heteroaryl, such as thiazolyl], were prepared for use in pharmaceutical compns. as glucokinase activators which are useful for treatment of type II diabetes. Thus, trans-cyclopropylcarboxamide II was prepared via an amidation reaction of the corresponding cyclopropanecarboxylic acid with (5-chlorothiazol-2-yl)amine hydrochloride using TBTU and Et3N in THF. The prepared cyclopropylcarboxamides were assayed for their ability to increase glucokinase activity. Also, pharmaceutical formulations containing the prepared cyclopropylcarboxamides were presented.
IT 731017-98-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted aryl substituted cyclopropylcarboxamides for therapeutic use as glucokinase activators)
RN 731017-98-4 CAPLUS
CN 2-Thiopheneacetic acid, 5-bromo-α-(cyclohexylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 16 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:454714 CAPLUS
DOCUMENT NUMBER: 141:174129
TITLE: A novel ring-opening reaction of (Z)-2-methyl-4-arylmethylene-5(4H)-oxazolone derivatives with acylhydrazines
AUTHOR(S): Maekawa, Kei; Kanno, Yoshitaka; Kubo, Kanji; Igarashi, Tetsutaro; Sakurai, Tadamitsu
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Kanagawa University, Yokohama, 221-8686, Japan
SOURCE: Heterocycles (2004), 63(6), 1273-1279
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:174129
AB The ring-opening mode of the title oxazolones with acylhydrazines was investigated from both the synthetic and mechanistic points of view. The reaction gives 1,3,4-triazole-substituted (Z)-α-dehydroamino acids in high yields, irresp. of substituents and solvents examined MM2 and PM5 calcns. strongly suggested that the triazole ring is constructed via the preferential nucleophilic addition of the hydrazino nitrogen to the C-N double bond in the oxazolone ring.
IT 733808-84-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(ring-opening reaction of (Z)-2-methyl-4-arylmethylene-5(4H)-oxazolones with acylhydrazines)
RN 733808-84-9 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3,5-dimethyl-α-(1-naphthalenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

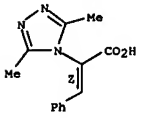
Double bond geometry as shown.



IT 733808-86-1P 733808-89-4P 733808-92-9P
733808-95-2P 733809-00-2P 733809-05-7P
733809-10-4P 733809-15-9P 733809-21-7P
733809-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ring-opening reaction of (Z)-2-methyl-4-arylmethylene-5(4H)-oxazolones with acylhydrazines)
RN 733808-86-1 CAPLUS

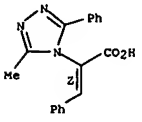
L4 ANSWER 16 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 4H-1,2,4-Triazole-4-acetic acid, 3,5-dimethyl-α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



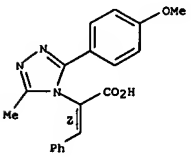
RN 733808-89-4 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-methyl-5-phenyl-α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 733808-92-9 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-(4-methoxyphenyl)-5-methyl-α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

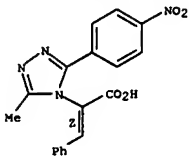
Double bond geometry as shown.



RN 733808-95-2 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-methyl-5-(4-nitrophenyl)-α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

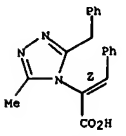
Double bond geometry as shown.

L4 ANSWER 16 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



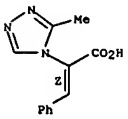
RN 733809-00-2 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-methyl-5-(phenylmethyl)-α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 733809-05-7 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-methyl-α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

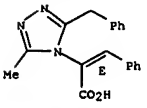
Double bond geometry as shown.



RN 733809-10-4 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3,5-dimethyl-α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

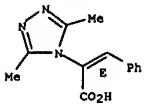
Double bond geometry as shown.

L4 ANSWER 16 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



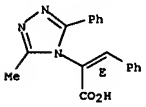
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 16 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



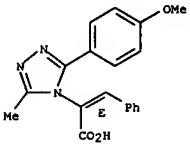
RN 733809-15-9 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-methyl-5-phenyl-α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 733809-21-7 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-(4-methoxyphenyl)-5-methyl-α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 733809-28-4 CAPLUS
CN 4H-1,2,4-Triazole-4-acetic acid, 3-methyl-5-(phenylmethyl)-α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

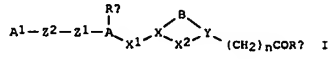
Double bond geometry as shown.

L4 ANSWER 17 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

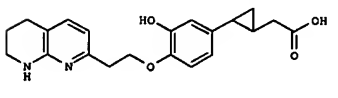
ACCESSION NUMBER: 2004:392322 CAPLUS
DOCUMENT NUMBER: 140:406797
TITLE: Preparation of heterocyclyl-substituted cycloalkylalkanoic acids as integrin receptor antagonists
INVENTOR(S): Nagarajan, Srinivasan R.; Khanna, Ish Kumar; Clare, Michael; Gasiecki, Alan; Rogers, Thomas; Chen, Barbara; Russell, Mark; Lu, Hwang-fun; Yi, Yu; Huff, Renee M.; Desai, Bipinchandra N.; Devadas, Balekudru; Parikh, Mihir D.; Penning, Thomas
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 96 pp., Cont.-in-part of U.S. Ser. No. 882,186.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004092538	A1	20040513	US 2002-326299		20021220
US 6921767	B2	20050726			
US 2002077321	A1	20020620	US 2001-882186		20010615
US 6900232	B2	20050531			
US 2004259869	A1	20041223	US 2004-891361		20040714
US 6949578	B2	20050927			
PRIORITY APPLN. INFO.:			US 2000-211781P	P	20000615
			US 2001-882186	A2	20010615

OTHER SOURCE(S): MARPAT 140:406797
GI



I



II

AB Title compds. I [wherein A = monocyclic or bicyclic ring; A1 = (un)substituted monocyclic or bicyclic heterocycle, NR5C(=Y1)NR7R8, etc.; X and Y = independently (un)substituted CH or N; X1 = O, CO, SO2, NH, N-alkyl, or (un)substituted (CH2)0-1; X2 = (un)substituted CH2 or NH, CO, SO2, O, or S; BXX2Y = (un)substituted monocyclic or bicyclic (hetero)cycle; Y1 = (un)substituted NH, O, or S; Z1 = CH2, O, NH, N-alkyl, CO, S, SO, or SO2; Z2 = 2-5 carbon linker optionally containing one or more heteroatoms; alternatively Z1Z2 may further contain a carboxamide,

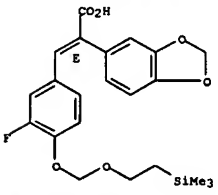
L4 ANSWER 17 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
sulfone, oxime, sulfonamide, alkenyl, alkynyl, or acyl group; Rb = (un)substituted OH, SH, or NH2; Rc = H, halo, OH, NO2, alkyl, alkoxy, NH2, (hetero)aryl, acyl(amino)sulfonyl, sulfonamide, CN, carboxamido, etc.; R5 = H or alkyl; R7 and R8 = independently H, (cyclo)alkyl, (alkyl)amino, OH, alkoxy, arylamino, amido, acyl, alkoxycarbonyl, aryloxy(carbonyl), benzoyl, aryl, etc.; or NR7R8 = (un)substituted heterocyclyl; n = 0-2; and pharmaceutically acceptable salts thereof] were prepd. for selectively inhibiting or antagonizing the αvβ3 and/or αvβ5 integrins (vitronectin receptors). For example, condensation of 2-(5,6,7,8-tetrahydro-1,9-naphthyridin-2-yl)-1-ethanol and Et (trans)-[2-(3,4-dihydroxyphenyl]cyclopropyl]acetate (7-step synthesis given) in the presence of polymer-bound PPh3 and diisopropyl azodicarboxylate in THF, followed by sapon. of the resulting ester using LiOH in MeCN/H2O, gave (trans)-II. In cell adhesion assays, compds. of the invention antagonized human αvβ3 and αvβ5 integrins with IC50 values of 0.1 nM to 100 μM and <50 μM, resp. Thus, I and their pharmaceutical compns. are useful for the treatment of tumor metastasis, solid tumor growth, angiogenesis, osteoporosis, humoral hypercalcemia of malignancy, smooth muscle cell migration, restenosis, atherosclerosis, macular degeneration, retinopathy, and arthritis (no data).

IT 689258-62-6P, (2E)-2-(1,3-Benzodioxol-5-yl)-3-[3-fluoro-4-[[2-(trimethylsilyl)ethoxy]methoxy]phenyl]prop-2-enoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of heterocyclyl-substituted cycloalkylalkanoic acids as αvβ3 and αvβ5 antagonists for treatment of tumors and other integrin-mediated conditions)

RN 689258-62-6 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[[3-fluoro-4-[[2-(trimethylsilyl)ethoxy]methoxy]phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 17 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:354796 CAPLUS
DOCUMENT NUMBER: 140:368653
TITLE: Endothelin receptor antagonist-EGF receptor tyrosine kinase inhibitor combination for the treatment of cancer
INVENTOR(S): Boyle, Francis Thomas; Curwen, Jon Owen; Gallagher, Neil James; Hancox, Ursula Joy; Hughes, Andrew Mark; Johnstone, Donna; Taylor, Sian Tomiko; Tonge, David William
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035057	A1	20040429	WO 2003-GB4347	20031007
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2501959	A1	20040429	CA 2003-2501959	20031007
AU 2003269259	A1	20040504	AU 2003-269259	20031007
EP 1553950	A1	20050720	EP 2003-751038	20031007
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003015140	A	20050816	BR 2003-15140	20031007
CN 1703224	A	20051130	CN 2003-80101310	20031007
JP 2006510605	T	20060330	JP 2004-544431	20031007
NO 2005001658	A	20050506	NO 2005-1658	20050404
ZA 2005002874	A	20060222	ZA 2005-2874	20050408
US 2006122180	A1	20060608	US 2005-530794	20050408
PRIORITY APPLN. INFO.:			GB 2002-23854 A	20021012
			WO 2003-GB4347 W	20031007

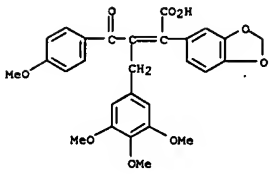
AB A combination, comprising an endothelin receptor antagonist (e.g. ZD4054), or a pharmaceutically acceptable salt thereof, and an EGF receptor tyrosine kinase inhibitor (e.g. ZD1839), or a pharmaceutically acceptable salt thereof, is described. The combination of the invention is useful for the treatment of cancer, e.g. prostate cancer.

IT 162412-70-6, PD 156707 162412-71-7, PD 155080
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin receptor antagonist-EGF receptor tyrosine kinase inhibitor combination for treatment of cancer)

RN 162412-70-6 CAPLUS

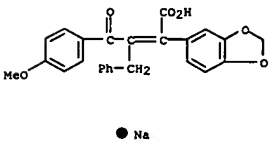
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA

L4 ANSWER 18 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)



RN 162412-71-7 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



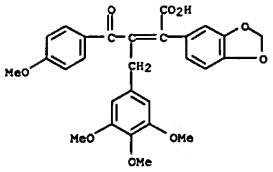
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:331974 CAPLUS
DOCUMENT NUMBER: 140:332519
TITLE: 5-HT1B/1D receptor agonists for the treatment of headache resulting from administering an endothelin receptor antagonist
INVENTOR(S): Curwen, Jon Owen; Hughes, Andrew Mark; Johnstone, Donna; Morris, Clive Dylan
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca Uk Limited
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004032922	A1	20040422	WO 2003-GB4338	20031006
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003274307	A1	20040504	AU 2003-274307	20031006
EP 1551395	A1	20050713	EP 2003-758297	20031006
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508933	T	20060316	JP 2004-542622	20031006
US 2006009512	A1	20060112	US 2005-530232	20050404
PRIORITY APPLN. INFO.:			GB 2002-23367 A	20021009
			WO 2003-GB4338 W	20031006

AB The invention discloses the use of a 5-HT1B/1D receptor agonist in the treatment or prevention of headache that results from administering an endothelin receptor antagonist. The invention also discloses a combination comprising an endothelin receptor antagonist and a 5-HT1B/1D receptor agonist.
IT 162412-70-6, PD 156707 162412-71-7, PD 155080
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(5-HT1B/1D receptor agonists for the treatment of headache resulting from administering an endothelin receptor antagonist)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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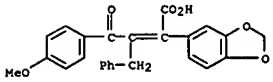
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



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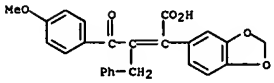
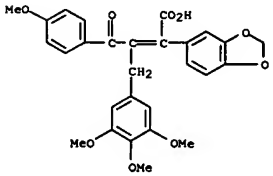
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:322089 CAPLUS
DOCUMENT NUMBER: 141:16897
TITLE: Chemical Function Based Pharmacophore Generation of Endothelin-A Selective Receptor Antagonists
AUTHOR(S): Funk, Oliver F.; Kettmann, Viktor; Drimal, Jan; Langer, Thierry
CORPORATE SOURCE: Department of Pharmaceutical, Chemistry Institute of Pharmacy, University of Innsbruck, Innsbruck, A-6020, Austria
SOURCE: Journal of Medicinal Chemistry (2004), 47(11), 2750-2760
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Both quant. and qual. chemical function based pharmacophore models of endothelin-A (ETA) selective receptor antagonists were generated by using the two algorithms HypoGen and HipHop, resp., which are implemented in the Catalyst mol. modeling software. The input for HypoGen is a training set of 18 ETA antagonists exhibiting IC50 values ranging between 0.19 nM and 67 μM. The best output hypothesis consists of five features: two hydrophobic (HY), one ring aromatic (RA), one hydrogen bond acceptor (HBA), and one neg. ionizable (NI) function. The highest scoring Hip Hop model consists of six features: three hydrophobic (HY), one ring aromatic (RA), one hydrogen bond acceptor (HBA), and one neg. ionizable (NI). It is the result of an input of three highly active, selective, and structurally diverse ETA antagonists. The predictive power of the quant. model could be approved by using a test set of 30 compds., whose activity values spread over 6 orders of magnitude. The two pharmacophores were tested according to their ability to extract known endothelin antagonists from the 3D mol. structure database of Derwent's World Drug Index. Thereby the main part of selective ETA antagonistic entries was detected by the two hypotheses. Furthermore, the pharmacophores were used to screen the Maybridge database. Six compds. were chosen from the output hit lists for in vitro testing of their ability to displace endothelin-1 from its receptor. Two of these are new potential lead compds. because they are structurally novel and exhibit satisfactory activity in the binding assay.
IT 207522-05-2 677009-36-8 697767-54-7
697767-55-8 697767-57-0 697767-58-1
697767-59-2 697767-61-6 697767-62-7
697767-64-9 697767-65-0 697767-67-2
697767-69-4 697767-70-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chemical function bsed pharmacophore generation of endothelin-A selective receptor antagonists)
RN 207522-05-2 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)

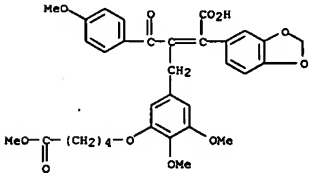
L4 ANSWER 20 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 677009-36-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

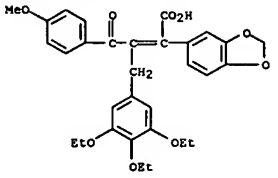


RN 697767-54-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-[(5-methoxy-5-oxopentyl)oxy]phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

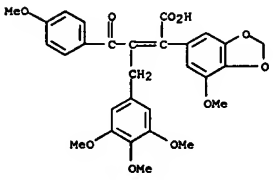


RN 697767-55-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-triethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

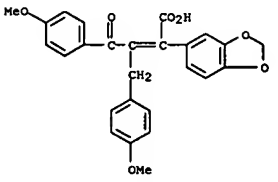
L4 ANSWER 20 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 697767-57-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

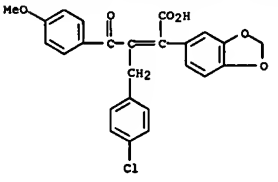


RN 697767-58-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-methoxyphenyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)

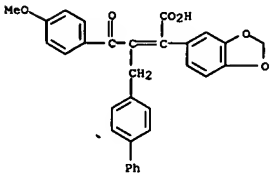


RN 697767-59-2 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-(cyclohexylmethyl)-2-(2,3-

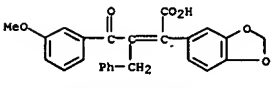
L4 ANSWER 20 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



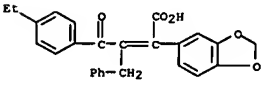
RN 697767-65-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-([1,1'-biphenyl]-4-ylmethyl)-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



RN 697767-67-2 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(3-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)

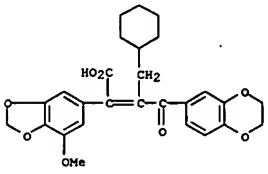


RN 697767-69-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-ethylphenyl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)

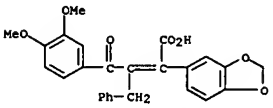


RN 697767-70-7 CAPLUS

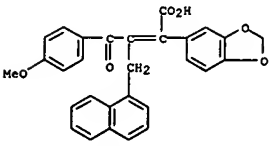
L4 ANSWER 20 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
dihydro-1,4-benzodioxin-6-yl)-2-oxoethylidene]-7-methoxy- (9CI) (CA INDEX NAME)



RN 697767-61-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(3,4-dimethoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)

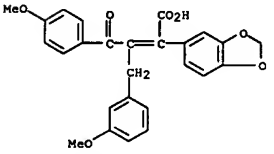


RN 697767-62-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-(1-naphthalenylmethyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



RN 697767-64-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(4-chlorophenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(3-methoxyphenyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



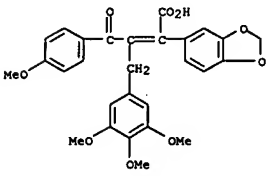
REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:291975 CAPLUS
DOCUMENT NUMBER: 140:315088
TITLE: Endothelin antagonists for treating Alzheimer's disease and dementias of vascular origin
INVENTOR(S): Gulati, Anil
PATENT ASSIGNEE(S): The Board of Trustees of the University of Illinois, USA
SOURCE: PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004028634	A1	20040408	WO 2003-US28212	20030910
WO 2004028634	A9	20040708		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003270446	A1	20040419	AU 2003-270446	20030910
US 2004092427	A1	20040513	US 2003-659579	20030910
PRIORITY APPLN. INFO.:			US 2002-413539P	P 20020925
			WO 2003-US28212	W 20030910

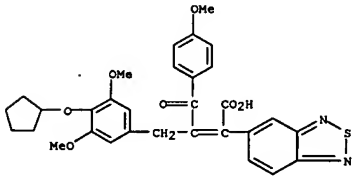
AB A composition and method of treating Alzheimer's disease or a dementia of vascular origin are disclosed. The composition and method utilize an endothelin antagonist as the active agent to treat Alzheimer's desease or a dementia of vascular origin in mammals, including humans.
IT 162412-70-6, PD 156707 219993-82-5 531491-66-4
677009-36-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin antagonists for treating Alzheimer's disease and vascular dementia)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



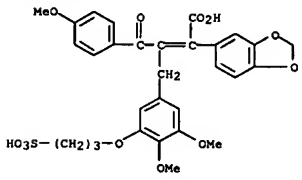
● Na

RN 219993-82-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

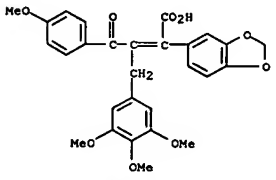


RN 531491-66-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-(3-sulfopropoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



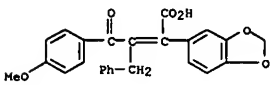
RN 677009-36-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:166465 CAPLUS
DOCUMENT NUMBER: 140:297200
TITLE: Effect of endothelin antagonism on contractility, intracellular calcium regulation and calcium regulatory protein expression in right ventricular hypertrophy of the rat
AUTHOR(S): Stessel, Heike; Brunner, Friedrich
CORPORATE SOURCE: Institute of Pharmacology and Toxicology, Karl-Franzens-University of Graz, Graz, A-8010, Austria
SOURCE: Basic & Clinical Pharmacology & Toxicology (2004), 94(1), 37-45
CODEN: BCPTBO; ISSN: 1742-7835
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have documented the effects of long-term endothelin receptor antagonism on intracellular Ca2+ regulation and Ca2+ regulatory protein expression in rat hearts with right ventricular hypertrophy without signs of heart failure. Rats were given either a single injection of monocrotaline (50 mg/kg, n=9) resulting in pulmonary hypertension-induced myocardial hypertrophy, or monocrotaline followed by daily administration of the endothelin subtype-A receptor antagonist 2-benzo(1,3)dioxol-5-yl-3-benzyl-4-(4-methoxy-phenyl-)-4-oxobut-2-enoate-Na (PD 155080, 50 mg/kg) over 9 wk (n=8). Hearts from saline-injected rats served as controls (n=9). Monocrotaline-treated animals developed marked right-sided hypertrophy without fibrosis as evident from hydroxyproline measurements, systolic contractility was increased, fully compensating for the increased afterload, but diastolic function was impaired as evident from protracted relaxation and slowed diastolic intracellular Ca2+ handling (measured by aequorin bioluminescence). In hypertrophic hearts, quant. immunoblotting analyses showed increased levels both of sarco(endo)plasmic reticulum Ca2+-ATPase (SERCA) and phosphorylated phospholamban, along with decreased levels of total phospholamban, which is in line with strengthened right ventricular systolic function. PD 155080 reversed abnormalities in Ca2+ handling, although SERCA and phospholamban protein levels were not altered (P=not significant vs. monocrotaline group). Thus, endothelin-A receptor antagonism attenuates right ventricular remodeling and improves myocardial Ca2+ handling, but has no discernable effect on elevated expression of SERCA and phospholamban observed in hypertrophic hearts. These data indicate that the hypotensive action of PD 155080 is independent of its effects, if any, on SERCA and its regulation.
IT 162412-71-7, PD 155080
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect of endothelin receptor antagonist PD155080 on contractility, intracellular calcium regulation and calcium regulatory protein expression in right ventricular hypertrophy of rat)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-

L4 ANSWER 22 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



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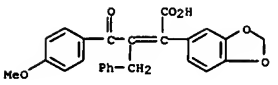
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:123801 CAPLUS
DOCUMENT NUMBER: 140:332965
TITLE: Cardiac effects of endothelin-1 (ET-1) and related C-terminal peptide fragment: increased inotropy or contribution to heart failure?
AUTHOR(S): Drimal, J.; Knezl, V.; Drimal, J., Jr.; Drimal, D.; Bauerova, K.; Kettmann, V.; Doherty, A. M.; Stefek, M.
CORPORATE SOURCE: Institute of Experimental Pharmacology, Slovak Academy of Sciences, Bratislava, Slovakia
SOURCE: Physiological Research (Prague, Czech Republic) (2003), 52(6), 701-708
CODEN: PHRSEJ; ISSN: 0862-8408
PUBLISHER: Institute of Physiology, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The contrasting pattern of cardiac inotropy induced by human peptide endothelin-1 (ET-1) has not been satisfactorily explained. It is not clear whether ET-1 is primarily responsible for increased myocardial ET-1 expression and release with resultant inotropic effects, or for the induction of myocardial hypertrophy and heart failure. There are at least two subtypes of endothelin receptors (ETA and ETB) and the inotropic effects of ET-1 differ depending on the receptor involved. Along with some other groups, we reported significant subtype-ETB endothelin receptor down-regulation in human cardiac cells preincubated with endothelin agonists (Drimal et al. 1999, 2000). The present study was therefore designed to clarify the subtype-selective mechanisms underlying the inotropic response to ET-1 and to its ETB-selective fragment (8-21)ET-1 in the isolated rat heart. The hearts were subjected to (1-21)ET-1 and to (8-21)ET-1, or to 30 min of stop-flow ischemia followed by 40 min of reperfusion, both before and after selective blockade of endothelin receptors. The present study revealed that both peptides, ET-1 and its (8-21)ET-1 fragment, significantly reduced coronary blood flow in nmolar and higher concns. The concomitant neg. inotropy and chronotropy were marked after ET-1, while the infusion of the ET-1(8-21) fragment produced a slight but significant pos. inotropic effect. Among the four endothelin antagonists tested in continuous infusion only the non-selective PD145065 and ETB1/B2-selective BQ788 (in μmolar concns.) slightly reduced the early contractile dysfunction of the heart induced by ischemia, whereas ETA-selective PD155080 partially protected the rat heart on reperfusion.
IT 162412-71-7, PD155080
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cardiac effects of endothelin-1 (ET-1) and related C-terminal peptide fragment in control and ischemic hearts)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

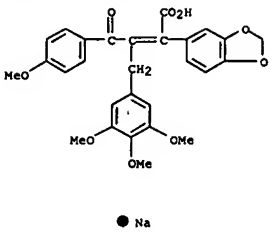
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:1007851 CAPLUS
DOCUMENT NUMBER: 140:53448
TITLE: Method and composition for potentiating the antipyretic action of a nonopioid analgesic
INVENTOR(S): Gulati, Anil
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 55 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003236235	A1	20031225	US 2003-459905	20030612
WO 2004000357	A1	20031231	WO 2003-US19151	20030617
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003279180	A1	20040106	AU 2003-279180	20030617
PRIORITY APPLN. INFO.:			US 2002-390045P	P 20020619
			WO 2003-US19151	W 20030617

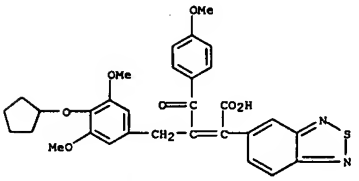
AB A composition and method of treating fever, and optionally treating pain, are disclosed. The composition and method utilize a non-opioid analgesic and an endothelin antagonist as active agents to treat fever in mammals, including humans. The composition also is useful in the prevention and treatment of stroke and other cardiovascular disorders, like myocardial infarction.
IT 162412-70-6, PD156707 219993-82-5 531491-66-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(method and composition for potentiating antipyretic action of nonopioid analgesic)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



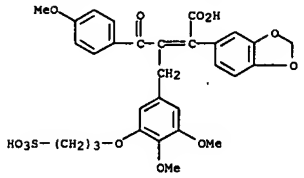
● Na

RN 219993-82-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



RN 531491-66-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-(3-sulfopropoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 25 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:414077 CAPLUS
DOCUMENT NUMBER: 139:957
TITLE: Method and composition using an endothelin antagonist for potentiating an opiate analgesic
INVENTOR(S): Gulati, Anil
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 55 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

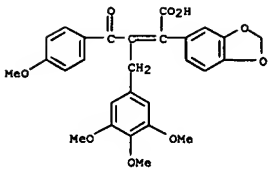
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003100507	A1	20030529	US 2002-301449	20021121
CA 2464768	A1	20030605	CA 2002-2464768	20021122
WO 2003045434	A2	20030605	WO 2002-US37461	20021122
WO 2003045434	A3	20030925		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002348224	A1	20030610	AU 2002-348224	20021122
EP 1448233	A2	20040825	EP 2002-782353	20021122
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002014481	A	20040914	BR 2002-14481	20021122
JP 2005513033	T	20050512	JP 2003-546935	20021122
CN 1646166	A	20050727	CN 2002-823570	20021122
ZA 2004003162	A	20050126	ZA 2004-3162	20040426
IN 2004CN01149	A	20060203	IN 2004-CN1149	20040526
NO 2004002612	A	20040622	NO 2004-2612	20040622
PRIORITY APPLN. INFO.:			US 2001-333599P P	20011127
			WO 2002-US37461 W	20021122

AB A composition and methods for treating pain and reducing or reversing tolerance to opiate analgesics are disclosed. The composition and methods use an opiate analgesic and an endothelin antagonist as active agents to treat pain in mammals, including humans.

IT 162412-70-6, PD 156707 219993-82-5 531491-66-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin antagonist for potentiation of opiate analgesic)

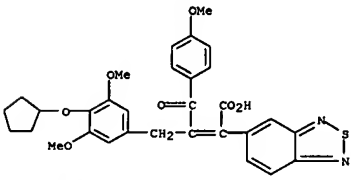
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

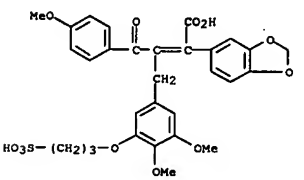


● Na

RN 219993-82-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



RN 531491-66-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-(3-sulfopropoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:376632 CAPLUS
DOCUMENT NUMBER: 138:379204
TITLE: Use of endothelin receptor antagonists in the treatment of tumor diseases
INVENTOR(S): Osswald, Mathias; Dorsch, Dieter; Mederski, Werner; Amendt, Christiane; Grell, Matthias
PATENT ASSIGNEE(S): Merck Patent GMBH, Germany
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003039539	A2	20030515	WO 2002-EP11350	20021010
WO 2003039539	A3	20031106		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10155076	A1	20030522	DE 2001-10155076	20011109
CA 2465744	A1	20030515	CA 2002-2465744	20021010
EP 1441721	A2	20040804	EP 2002-802624	20021010
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002013684	A	20041026	BR 2002-13684	20021010
CN 1585636	A	20050223	CN 2002-822252	20021010
HU 200402281	A2	20050228	HU 2004-2281	20021010
JP 2005510511	T	20050421	JP 2003-541830	20021010
US 2005014769	A1	20050120	US 2004-495108	20040510
ZA 2004004544	A	20050208	ZA 2004-4544	20040608
PRIORITY APPLN. INFO.:			DE 2001-10155076 A	20011109
			WO 2002-EP11350 W	20021010

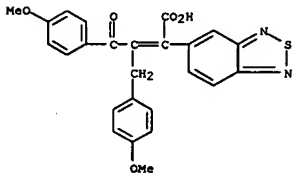
OTHER SOURCE(S): MARPAT 138:379204

AB The invention discloses the use of endothelin receptor antagonists in the production of a medicament for treating tumors.

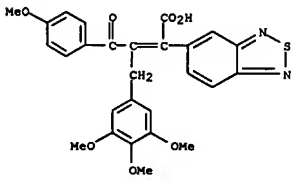
IT 195505-54-5 195506-97-9 195506-98-0
195507-00-7 209345-15-3 209345-16-4
219993-82-5 219993-83-6 525598-31-6
525598-32-7 525598-33-8 525598-34-9
525598-35-0 525598-38-3 525598-39-4
525598-40-7 525598-41-8 525598-47-4
525598-57-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(endothelin receptor antagonists for treatment of tumors)

RN 195505-54-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-methoxyphenyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)

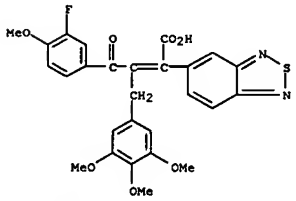


RN 195506-97-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

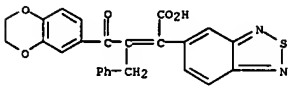


RN 195506-98-0 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 195507-00-7 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)



RN 209345-15-3 CAPLUS
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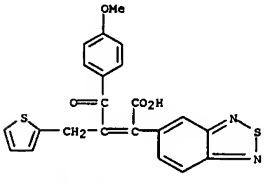
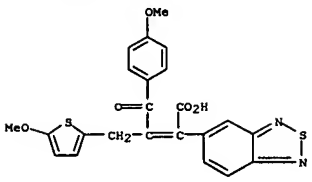
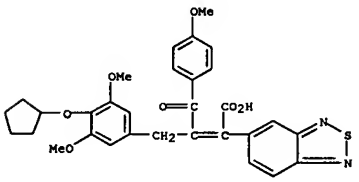


RN 209345-16-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(5-methoxy-2-thienyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)

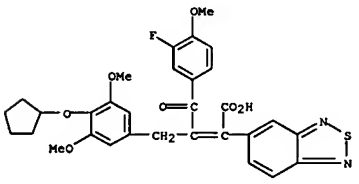
L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



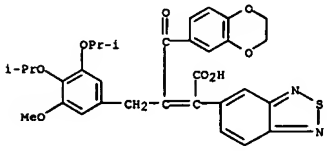
RN 219993-82-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



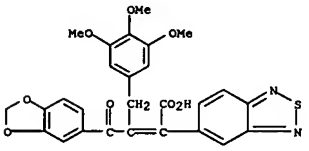
RN 219993-83-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(3-fluoro-4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



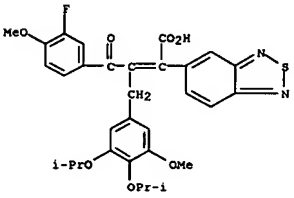
L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 525598-35-0 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(1,3-benzodioxol-5-yl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)



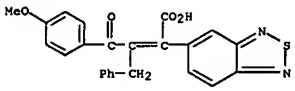
RN 525598-38-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-1-[[3-methoxy-4,5-bis(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



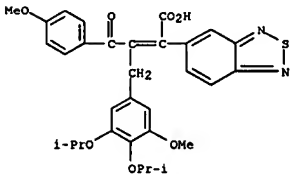
RN 525598-39-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3,5-dimethoxy-4-(1-methylethoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

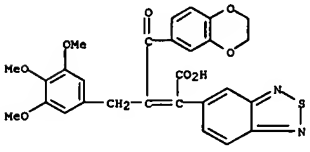
RN 525598-31-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)



RN 525598-32-7 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3-methoxy-4,5-bis(1-methylethoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

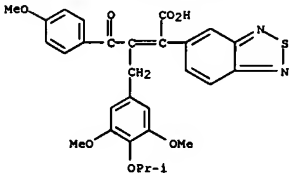


RN 525598-33-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

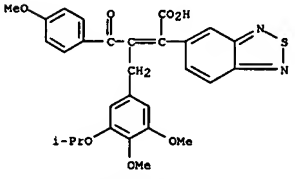


RN 525598-34-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-[[3-methoxy-4,5-bis(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)

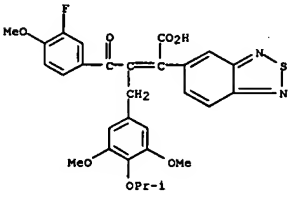
L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 525598-40-7 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-(1-methylethoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

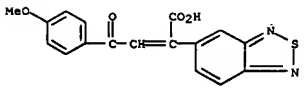


RN 525598-41-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3,5-dimethoxy-4-(1-methylethoxy)phenyl]methyl]-2-(3-fluoro-4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

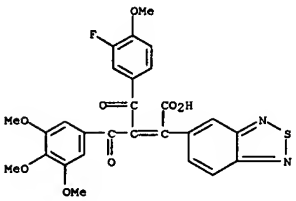


RN 525598-47-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-

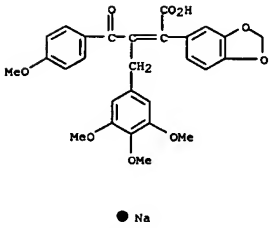
L4 ANSWER 26 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
oxoethylidene]- (9CI) (CA INDEX NAME)



RN 525598-57-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-(3-fluoro-4-methoxybenzoyl)-2-oxo-2-(3,4,5-trimethoxyphenyl)ethylidene]- (9CI) (CA INDEX NAME)



L4 ANSWER 27 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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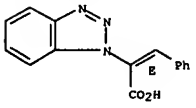
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 27 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:52507 CAPLUS
DOCUMENT NUMBER: 139:17349
TITLE: Antiarrhythmic effect of endothelin-A receptor antagonist on acute ischemic arrhythmia in isolated rat heart
AUTHOR(S): Xu, Hong; Lin, Li; Yuan, Wen-Jun
CORPORATE SOURCE: Department of Physiology, Second Military Medical University, Shanghai, 200433, Peop. Rep. China
SOURCE: Acta Pharmacologica Sinica (2003), 24(1), 37-44
CODEN: APSCG5; ISSN: 1671-4083
PUBLISHER: Science Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Aim: To observe the effects of endothelin receptor subtype A (ETA) and B (ETB) antagonists on acute ischemic arrhythmia in isolated rat heart, and to determine whether endogenous endothelin (ET) was implicated in the pathophysiol. process of arrhythmia induced by acute myocardial ischemia. Methods: Fifty-three SD male rats were randomized into 8 groups. Heart was isolated and perfused in Langendorff mode and acute ischemia model was established by ligation of the left anterior descending (LAD) coronary artery. The effects of ETA receptor antagonist PD156707 and ETB receptor antagonist IRL1038 on arrhythmia, heart function, the myocardial activity of superoxide dismutase (SOD), and the content of melondialdehyde (MDA) during the acute 60-min ischemic phase were analyzed. Results: Pretreatment with PD156707 (20-500 nmol/L) dose-dependently improved the ischemic isolated heart function, enhanced SOD activity and decreased MDA content in the ischemic myocardium, and suppressed the acute ischemic arrhythmia. Conversely pretreatment with IRL1038 did not change the heart function, SOD activity, MDA content, and the acute ischemic arrhythmia significantly as compared with the occlusion control. Conclusion: ETA receptor antagonist effectively improved heart function, enhanced anti-oxidative function of the myocardium and reduced arrhythmia during the acute ischemic phase in isolated rat hearts, while ETB receptor antagonist did not exert protective effects, suggesting that endogenous ET-1, acting through ETA receptor, may be one of the factors implicated in arrhythmia and impairment to heart function during the acute ischemic phase.
IT 162412-70-6, PD156707
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin receptor antagonists effect on acute ischemic arrhythmia and ET role)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 28 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:879145 CAPLUS
DOCUMENT NUMBER: 138:353896
TITLE: Synthesis and antiproliferative activity of 3-aryl-2-(1H-benzotriazol-1-yl)acrylonitriles. Part III
AUTHOR(S): Carta, Antonio; Sanna, Paolo; Palomba, Michele; Vargiu, Laura; La Colla, Massimiliano; Loddo, Roberta
CORPORATE SOURCE: Dipartimento Farmaco-Chimico-Tossicologico, Universita degli Studi di Sassari, Sassari, 07100, Italy
SOURCE: European Journal of Medicinal Chemistry (2002), 37(11), 891-900
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:353896
AB A new series of 30 3-aryl-2-(1H-benzotriazol-1-yl)acrylonitriles were synthesized and tested for biol. activity as part of our research in the antimicrobial and antitumor fields. In particular, title compds. were evaluated in vitro against representative strains of Gram-pos. and Gram-neg. bacteria (S. aureus, Salmonella spp), mycobacteria (M. fortuitum, M. smegmatis ATCC 19420 and M. tuberculosis ATCC 27294), yeast and mold (C. albicans ATCC 10231 and A. fumigatus). Furthermore, their antiretroviral activity against HIV-1 was determined in MT-4 cells together with cytotoxicity. In these assays title compds. and 47 addnl. derivs. described previously (P. Sanna, A. Carta, M.E. Rahbar Nikookar, Eur. J. Med. Chemical 35 (2000) 535-543; P. Sanna, A. Carta, L. Gherardini, M.E. Rahbar Nikookar, Farmaco 57 (2002) 79-87) were tested for their capability to prevent MT-4 cell growth. All compds. resulted devoid of antibacterial, antifungal and anti-HIV-1 activity. In anti-mycobacterial assays several compds. resulted active (MIC50=6.0-70 μM) against M. tuberculosis. However, since they showed cytotoxicity against MT-4 cells at lower concns. (CC50=0.05-25 μM), their anti-mycobacterial activity was not selective. For this reason, the most cytotoxic compds. were also evaluated for antiproliferative activity against a panel of human cell lines derived from both hematol. and solid tumors. Compound 34 resulted the most potent compound against the above human tumor-derived cell lines.
IT 445496-72-0 445496-73-1 445496-74-2
445496-75-3
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation and antiproliferative, antimycobacterial (antitubercular), anti-HIV-1, and antitumor activities of (aryl)(benzotriazolyl)acrylonitriles and their acyl derivs.)
RN 445496-72-0 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

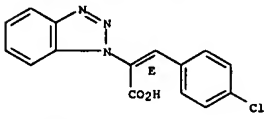
Double bond geometry as shown.

L4 ANSWER 28 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



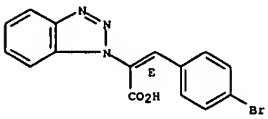
RN 445496-73-1 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-[(4-chlorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 445496-74-2 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-[(4-bromophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

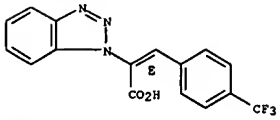
Double bond geometry as shown.



RN 445496-75-3 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-[[4-(trifluoromethyl)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

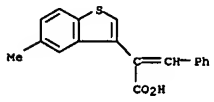
Double bond geometry as shown.

L4 ANSWER 28 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

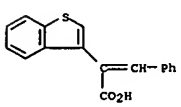


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:861050 CAPLUS
DOCUMENT NUMBER: 139:164660
TITLE: Product class 6: dibenzothiophenes
AUTHOR(S): Andrews, M. D.
CORPORATE SOURCE: Pfizer Central Research, Kent, CT13 9NJ, UK
SOURCE: Science of Synthesis (2001), 10, 211-263
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Methods for preparing dibenzothiophenes are reviewed including cyclization, ring transformation, aromatization and substituent modifications.
IT 83821-47-0P 183018-47-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dibenzothiophenes via cyclization, ring transformation, aromatization and substituent modifications)
RN 83821-47-0 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, 5-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



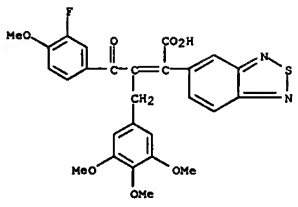
RN 183018-47-5 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 187 THERE ARE 187 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 30 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:852671 CAPLUS
DOCUMENT NUMBER: 138:219368
TITLE: Endothelin-A Receptor Blockade in Porcine Pulmonary Hypertension
AUTHOR(S): Ambalavanan, Namasivayam; Philips, Joseph B.; Bulger, Arlene; Oparil, Suzanne; Chen, Yiu-Fai
CORPORATE SOURCE: Departments of Pediatrics, University of Alabama at Birmingham, Birmingham, AL, 35233, USA
SOURCE: Pediatric Research (2002), 52(6), 913-921
CODEN: PEREBL; ISSN: 0031-3998
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Endothelin-1 can cause pulmonary vasoconstriction via endothelin-A (ETA) receptor activation. We hypothesized that ETA blockers (EMD 122946 and BQ 610) would reduce hypoxia-induced (HYP) but not group B streptococcal infusion (GBS)-induced pulmonary hypertension in a juvenile whole animal model. Pulmonary hypertension was created by exposing chronically instrumented piglets to HYP (n = 12) or heat-killed GBS (n = 11). ETA blockade was produced by increasing bolus doses of EMD122946 or BQ 610. Pulmonary arterial pressure (PAP), systemic arterial pressure (SAP), left atrial pressure, central venous pressure, and cardiac output were continuously measured. Pulmonary and systemic vascular resistance indexes (PVRI and SVRI) were calculated HYP doubled PAP and PVRI. Both ETA blockers decreased PAP and PVRI in a dose-dependent manner in HYP, with high doses decreasing PVRI to baseline and reducing PAP by 50%. GBS also doubled both PAP and PVRI. EMD 122946 did not change PAP or PVRI in GBS, although BQ 610 markedly increased PVRI (>100% increase with 0.15 mg/kg) and showed a trend toward increasing PAP. Both models showed minimal (<25%) changes in SAP or SVRI. Neither ETA blocker changed baseline hemodynamics in the absence of HYP or GBS. Pao2 did not change with GBS but decreased with BQ 610. ETA receptor blockade attenuated hypoxic, but not GBS induced pulmonary hypertension. BQ 610 worsened PVRI and oxygenation in the GBS model. Differences in response to ETA blockade in pulmonary hypertension may be seen depending on the etiol. (hypoxia vs. infection-associated), and the specific ETA antagonist used.
IT 195505-94-3, EMD122946
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ETA receptor blockade attenuates hypoxic but not group B streptococcal infusion induced pulmonary hypertension in piglet)
RN 195505-94-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 30 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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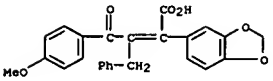
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 31 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 31 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:835405 CAPLUS
DOCUMENT NUMBER: 138:395779
TITLE: Long-term effects of selective and nonselective endothelin receptor antagonists in mice with heart failure
AUTHOR(S): Cavasin, Maria A.; Carretero, Oscar A.; Yang, Fang; Oja-Tebbe, Nancy; Peng, Hongmei; Yang, Xiao-Ping
CORPORATE SOURCE: Hypertension and Vascular Research Division, Henry Ford Health System, Detroit, MI, USA
SOURCE: Journal of Cardiac Failure (2002), 8(4), 254-261
CODEN: JCFAF9; ISSN: 1071-9164
PUBLISHER: Churchill Livingstone
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Background: The ETA and ETB receptors mediate vasoconstriction, aldosterone release, and fibrosis. However, the role of ETA receptors is still controversial because those expressed on endothelial cells also stimulate vasodilatation and may oppose the actions of the ETA receptor. Plasma levels of endothelin-1 (ET-1) are increased in heart failure (HF) and are associated with myocardial dysfunction. The relative efficacy of selective and nonselective ET antagonists in the treatment of HF is unclear. We hypothesized that blockade of ETA receptors may improve cardiac function and prevent left ventricular remodeling in mice with HF and these effects may be mediated in part by activation of ETB. Methods and Results: A mouse model of chronic HF induced by myocardial infarction (MI) was used. Seven days after MI, mice were divided into vehicle, ETA-ant (antagonist), or ETA/B-ant groups and treated for 23 wk. Cardiac function, LV dimensions, and hemodynamics were evaluated in conscious mice before MI and during treatment. Histol. anal. of the heart and liver was performed at the end of the study. HF significantly decreased EF and increased LV dimensions, interstitial collagen fraction (ICF) and myocyte cross-sectional area (MCSA). Both ETA-ant and ETA/B-ant slightly increased EF but had no significant effect on LV dimensions, hypertrophy, or ICF. Both treatments decreased MCSA; however, this was only significant in the ETA/B-ant group. Conclusions: Both selective and nonselective ET-ant have similar slight effects on cardiac function and remodeling. This suggests that (1) ETB receptors do not mediate the beneficial cardiac effects of ETA-ant and (2) blockade of the ET system alone may not provide significant cardioprotection, at least in mice with HF induced by MI.

IT 162412-71-7, PD 155080
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); BIOL (Biological study)
(endothelin receptor selective and nonselective antagonists long-term effects in mice with heart failure induced by infarction)

RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

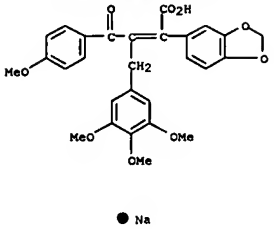
ACCESSION NUMBER: 2002:816291 CAPLUS
DOCUMENT NUMBER: 138:331439
TITLE: ETA receptor antagonists inhibit intimal smooth muscle cell proliferation in human vessels
AUTHOR(S): Maguire, Janet J.; Yu, Julie C.-M.; Davenport, Anthony P.
CORPORATE SOURCE: Clinical Pharmacology Unit, University of Cambridge, Cambridge, CB2 2QQ, UK
SOURCE: Clinical Science (2002), 103(Suppl.), 184S-188S
CODEN: CSCIAE; ISSN: 0143-5221
PUBLISHER: Portland Press Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have determined the ability of the endothelin (ET)A receptor antagonist, PD 156707 (CI 1020), to inhibit intimal proliferation in human saphenous veins maintained in organ culture. After 28 days in culture, veins exposed to 1 μM PD 156707 exhibited a significant reduction in intima to intima-plus-media ratio (1:1+M ratio) (0.14) and an increase in lumen area (3.1 mm2) compared with veins cultured without the antagonist (1:1+M, 0.29; lumen area, 2.5 mm2) but were not significantly different from precultured controls (1:1 + M, 0.15; lumen area, 4.4 mm2) (Dunn's test for non-parametric multiple comparisons: $\alpha < 0.05$). In organ bath expts., ET-1 and 5-hydroxytryptamine constricted precultured control vessels with pD2 values (where pD2 is defined as the neg. logarithm of the molar EC50 value of an agonist) of 8.9 and 7.0 and Emax (efficacy) values of 86% and 71% (compared with constriction induced by KCl) resp. There was no difference in the responsiveness of veins cultured for 14 days to either agonist, indicating that the vessels maintained in organ culture remain viable. Crucially, vein segments cultured with 1 μM PD 156707 (a concentration that antagonized ET-1 responses in precultured control vessels) contracted to ET-1 with a potency comparable to that obtained in vessels cultured in the absence of the antagonist (pD2 = 8.9 and 8.0 resp.) confirming that PD 156707 was not toxic to the tissue at the concentration used.
In conclusion we have shown that the ETA-selective antagonist, PD 156707, completely blocked intimal hyperplasia in human saphenous veins in organ culture, suggesting that ETA antagonists may be beneficial in preventing or delaying saphenous vein graft disease in patients receiving bypass grafts for coronary artery disease.

IT 162412-70-6, PD 156707
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin ETA receptor antagonists inhibit intimal smooth muscle cell proliferation in human vessels)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 33 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:733842 CAPLUS
DOCUMENT NUMBER: 137:252999
TITLE: Inhalant drug delivery systems composed of anticholinergics and endothelin antagonists
INVENTOR(S): Montague, Meade Christopher J.; Pairet, Michel; Pieper, Michael P.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma KG, Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10113366	A1	20020926	DE 2001-10113366	20010320
CA 2441964	A1	20020926	CA 2002-2441964	20020307
WO 2002074034	A2	20020926	WO 2002-EP2494	20020307
WO 2002074034	A3	20031023		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002254930	A1	20021003	AU 2002-254930	20020307
EP 1379225	A2	20040114	EP 2002-724207	20020307
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004525920	T	20040826	JP 2002-572762	20020307
US 2002183347	A1	20021205	US 2002-100659	20020318
US 6608054	B2	20030819		
US 2003203925	A1	20031030	US 2003-413065	20030414
US 2005148562	A1	20050707	US 2004-6940	20041208

PRIORITY APPLN. INFO.:

DE 2000-10054042	A	20001031
US 2000-253613P	P	20001128
DE 2000-10062712	A	20001215
DE 2000-10063957	A	20001220
US 2000-257220P	P	20001221
US 2000-257221P	P	20001221
DE 2001-10110772	A	20010307
DE 2001-10111058	A	20010308

L4 ANSWER 33 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

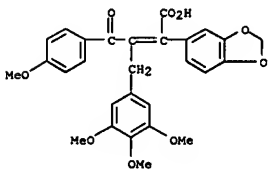
DE 2001-10113366	A	20010320
US 2001-281653P	P	20010405
US 2001-281857P	P	20010405
US 2001-281874P	P	20010405
DE 2001-10138272	A	20010810
US 2001-314599P	P	20010824
US 2001-7182	B1	20011019
US 2001-86145	B1	20011019
US 2001-27662	B1	20011220
DE 2002-10206505	A	20020216
US 2002-92116	A1	20020306
US 2002-93240	B1	20020307
WO 2002-EP2494	W	20020307
US 2002-100659	A1	20020318
US 2002-369213P	P	20020401
US 2003-360064	A2	20030207
US 2003-413065	B2	20030414
US 2003-419358	A1	20030421
US 2003-613783	A2	20030703
US 2004-763894	A2	20040123
US 2004-775901	A2	20040210
US 2004-776757	A2	20040211
US 2004-824391	A2	20040414

AB The invention concerns inhalants for the treatment of respiratory diseases that contain anticholinergics and endothelin antagonists; the inhalants can be dosed with or without propellants and can contain excipients. Anticholinergics are salts of tiotropium, oxitropium and ipratropium; endothelin antagonists are selected from the group of Tezosentan, Bosentan, Enrasentan, Sixtasentan, T-0201, BMS-193884, K-8794, PD-156123, PD-156707, PD-160874, PD-180988, S-0139 and ZD-1611. Thus an inhalant powder was composed of capsules that contained per capsule (μg): tiotropium bromide 21.7; endothelin antagonist 270; lactose 4708.3.

IT 162412-70-6, PD-156707
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhalant drug delivery systems composed of anticholinergics and endothelin antagonists)

L4 ANSWER 33 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

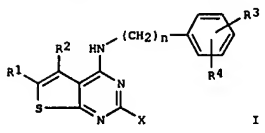
L4 ANSWER 34 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:591553 CAPLUS
DOCUMENT NUMBER: 137:154940
TITLE: Preparation of thieno[2,3-d]pyrimidines as inhibitors of cGMP- and cAMP-phosphodiesterase (PDE V)
INVENTOR(S): Eggenweiler, Hans-Michael; Eiermann, Volker; Schelling, Pierre
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10104802	A1	20020808	DE 2001-10104802	20010202
CA 2437085	A1	20020815	CA 2002-2437085	20020114
WO 2002062343	A2	20020815	WO 2002-EP256	20020114
WO 2002062343	A3	20021121		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002235832	A1	20020819	AU 2002-235832	20020114
EP 1357915	A2	20031105	EP 2002-702259	20020114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 200303005	A2	20031229	HU 2003-3005	20020114
BR 2002006853	A	20040113	BR 2002-6853	20020114
JP 2004525890	T	20040826	JP 2002-562350	20020114
US 2004063731	A1	20040401	US 2003-470763	20030731
IN 2003KN01085	A	20050708	IN 2003-KN1085	20030827

PRIORITY APPLN. INFO.:
DE 2001-10104800 A 20010202
DE 2001-10104801 A 20010202
DE 2001-10104802 A 20010202
WO 2002-EP256 W 20020114

OTHER SOURCE(S): MARPAT 137:154940
GI

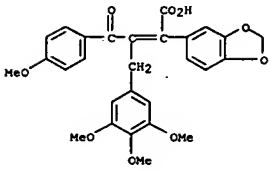
L4 ANSWER 34 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

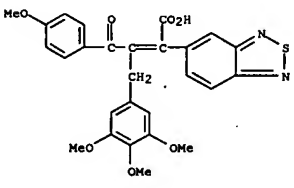
AB Pharmaceutical formylation containing title compds. [I; R1, R2 = H, A, halo; or R1R2 = C3-5 alkylene; R3,R4 = H, A, OA, OH, halo; or R3R4 = C3-5 alkylene , OCH2CH2, OCH2O, OCH2CH2O; X = (CO2H-, CO2A-, CONH2-, CONHA-, CONA2-, cyano-substituted) (interrupted) alkylene, cycloalkylalkylene, C6H4(CH2)m; A = C1-6 alkyl; m = 1, 2; n = 0-3] and/or salts, and/or solvates thereof, and ≥1 endothelin receptor antagonist, is claimed. Thus, 2.2 g Me 3-[4-(3-chloro-4-methoxybenzylamino)-5,6,7,8-tetrahydro-[1]benzothieno[2,3-d]pyrimidin-2-yl]propionate (preparation given) was saponified with 32% NaOH to 2.0 g the corresponding propionic acid which was crystallized with HOCH2CH2NH2 to give 1.35 g 3-[4-(3-chloro-4-methoxybenzylamino)-5,6,7,8-tetrahydro-[1]benzothieno[2,3-d]pyrimidin-2-yl]propionic acid ethanolamine salt. I were said to show affinity for cGMP- and cAMP-phosphodiesterase (PDE V) (no data).
IT 162412-70-6, Pd-156707 195505-82-9, Emd-122801
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin receptor antagonist; for pharmaceutical formylation containing thienopyrimidines as inhibitors of cGMP- and cAMP-phosphodiesterase (PDE V))
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 34 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 195505-82-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

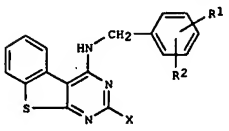
L4 ANSWER 35 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:591552 CAPLUS
DOCUMENT NUMBER: 137:154939
TITLE: Preparation of 4-benzylamino[1]benzothieno[2,3-d]pyrimidines as inhibitors of cGMP- and cAMP-phosphodiesterase (PDE V)
INVENTOR(S): Eggenweiler, Hans-Michael; Eiermann, Volker; Schelling, Pierre
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 38 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10104801	A1	20020808	DE 2001-10104801	20010202
CA 2437085	A1	20020815	CA 2002-2437085	20020114
WO 2002062343	A2	20020815	WO 2002-EP256	20020114
WO 2002062343	A3	20021121		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002235832	A1	20020819	AU 2002-235832	20020114
EP 1357915	A2	20031105	EP 2002-702259	20020114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 200303005	A2	20031229	HU 2003-3005	20020114
BR 2002006853	A	20040113	BR 2002-6853	20020114
JP 2004525890	T	20040826	JP 2002-562350	20020114
US 2004063731	A1	20040401	US 2003-470763	20030731
IN 2003KN01085	A	20050708	IN 2003-KN1085	20030827

PRIORITY APPLN. INFO.:
DE 2001-10104800 A 20010202
DE 2001-10104801 A 20010202
DE 2001-10104802 A 20010202
WO 2002-EP256 W 20020114

OTHER SOURCE(S): MARPAT 137:154939
GI

L4 ANSWER 35 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

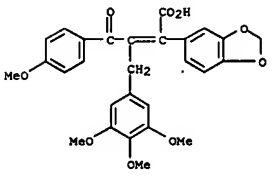
AB Pharmaceutical formylation containing title compds. [I; R1, R2 = H, A, OA, OH, halo; or R1R2 = C3-5 alkylene, OCH2CH2, CH2OCH2, OCH2O, OCH2CH2O; X = (CO2H-, CO2A-, CONH2-, CONHA-, CONA2-, cyano-substituted) (interrupted) alkylene, cycloalkyl, cycloalkylalkylene, Ph, PhMe; A = C1-6 alkyl] and/or salts, and/or solvates thereof, and ≥1 endothelin receptor antagonist, is claimed. Thus, Me 4-(4-chlorobenzothieno[2,3-d]pyrimidin-2-yl)phenylcarboxylic acid ester was heated at 110° with 3-chloro-4-methoxybenzylamine in N-methylpyrrolidone for 4 h to give ca. 61% Me 4-[4-(3-chloro-4-methoxybenzylamino)[1]benzothieno[2,3-d]pyrimidin-2-yl]benzoate. I were said to show affinity for cGMP- and cAMP-phosphodiesterase (PDE V) (no data).

IT 162412-70-6, Pd-156707 195505-82-9, Emd-122801
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin receptor antagonist; for pharmaceutical formylation containing benzothienopyrimidines as inhibitors of cGMP- and cAMP-phosphodiesterase (PDE V))

RN 162412-70-6 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

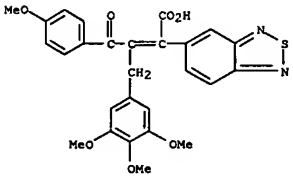
L4 ANSWER 35 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 195505-82-9 CAPLUS

CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

L4 ANSWER 36 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:591551 CAPLUS
DOCUMENT NUMBER: 137:154938
TITLE: Preparation of pyrazolo[4,3-d]pyrimidines as inhibitors of cGMP- and cAMP-phosphodiesterase (PDE V)
INVENTOR(S): Eggenweiler, Hans-Michael; Eiermann, Volker; Schelling, Pierre
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 38 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10104800	A1	20020808	DE 2001-10104800	20010202
CA 2437085	A1	20020815	CA 2002-2437085	20020114
WO 2002062343	A2	20020815	WO 2002-EP256	20020114
WO 2002062343	A3	20021121		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002235832	A1	20020819	AU 2002-235832	20020114
EP 1357915	A2	20031105	EP 2002-702259	20020114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 200303005	A2	20031229	HU 2003-3005	20020114
BR 2002006853	A	20040113	BR 2002-6853	20020114
JP 2004525890	T	20040826	JP 2002-562350	20020114
US 2004063731	A1	20040401	US 2003-470763	20030731
IN 2003KN01085	A	20050708	IN 2003-KN1085	20030827
ZA 2003006819	A	20041201	ZA 2003-6819	20030901

PRIORITY APPLN. INFO.:
DE 2001-10104800 A 20010202
DE 2001-10104801 A 20010202
DE 2001-10104802 A 20010202
WO 2002-EP256 W 20020114

OTHER SOURCE(S): MARPAT 137:154938
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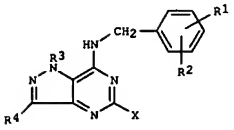
L4 ANSWER 36 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



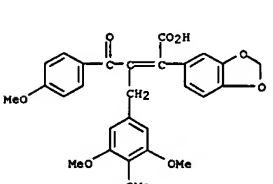
I

AB Pharmaceutical formylation containing title compds. [I; R1, R2 = H, A, OA, OH, halo; or R1R2 = C3-5 alkylene, OCH2CH2, CH2OCH2, OCH2O, OCH2CH2O; R3, R4 = H, A; X = (CO2H-, CO2A-, CONH2-, CONHA-, CONA2-, cyano-substituted) (interrupted) alkylene, cycloalkyl, cycloalkylalkylene, Ph, PhMe; A = C1-6 alkyl] and/or salts, and/or solvates thereof, and ≥1 endothelin receptor antagonist, is claimed. Thus, Me 4-[7-chloro-1-methyl-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl]phenylcarboxylic acid ester was heated at 110° with 3-chloro-4-methoxybenzylamine in N-methylpyrrolidone for 4 h to give ca. 54% Me 4-[7-(3-chloro-4-methoxybenzylamino)-1-methyl-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl]benzoate. I were said to show affinity for cGMP- and cAMP-phosphodiesterase (PDE V) (no data).

IT 162412-70-6, Pd-156707 195505-82-9, Emd-122801
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin receptor antagonist; for pharmaceutical formylation containing pyrazolopyrimidines as inhibitors of cGMP- and cAMP-phosphodiesterase (PDE V))

RN 162412-70-6 CAPLUS

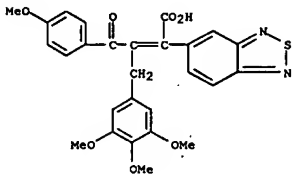
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

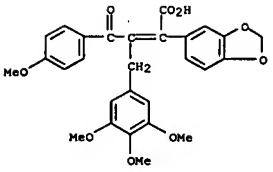
L4 ANSWER 36 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 195505-82-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

L4 ANSWER 37 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

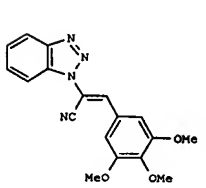
L4 ANSWER 37 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:567358 CAPLUS
DOCUMENT NUMBER: 138:147475
TITLE: The endothelin A receptor antagonists PD 156707 (Cl-1020) and PD 180988 (Cl-1034) reverse the hypoxic pulmonary vasoconstriction in the perinatal lamb
AUTHOR(S): Coe, Yashu; Haleen, Stephen J.; Welch, Kathleen M.; Liu, You-An; Coceani, Flavio
CORPORATE SOURCE: Department of Paediatrics, University of Alberta, Edmonton, AB, Can.
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2002), 302(2), 672-680
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Endothelin-1 (ET-1) is considered an intermediary in the constrictor response of the pulmonary vasculature to hypoxia and, by extension, is assigned a prime role in the pathogenesis of pulmonary hypertension. We report here the antihypertensive action in the conscious newborn lamb of two novel endothelin A receptor antagonists, sodium 2-benzo-[1,3]dioxol-5-yl-4-(4-methoxyphenyl)-4-oxo-3-(3,4,5-trimethoxybenzyl)-but-2-enoate (PD 156707) and 4-(7-ethyl-benzo[1,3]dioxol-5-yl)-1,1-dioxo-2-(2-trifluoromethylphenyl)-1, 2-dihydro-1l6-benzo-[e][1,2]thiazine-3-carboxylic acid potassium (PD 180988), differing in chemical properties and half-life within the body. PD 156707 and PD 180988, given in the right atrium as a bolus followed by infusion, had little or no effect on pulmonary and systemic hemodynamics under normoxia. Conversely, they both reversed the pulmonary hypertension due to alveolar hypoxia while producing minor changes, or no change at all, in systemic vascular resistance. Furthermore, their pulmonary vascular effect outlasted administration. Pulmonary hypertension being elicited by infusion of the thromboxane A2 analog, 9,11-epithio-11,12-methano-thromboxane A2 (ONO-11113) was instead not amenable to ETAR inhibition. Blood levels of ET-1, which rose with hypoxia but not ONO-11113 treatment, were not changed by either antagonist. Consistent with findings in vivo, when using isolated pulmonary resistance arteries from term fetal lamb, PD 156707 curtailed the hypoxia- but not the ONO-11113-induced constriction. We conclude that PD 156707 and PD 180988 are selective inhibitors of pulmonary vasoconstriction resulting from hypoxia. Our findings support the use of these or allied compds. in the management of pulmonary hypertension in the neonate.

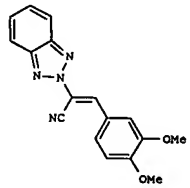
IT 162412-70-6, PD 156707
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin A antagonists PD 156707 and PD 180988 reverse hypoxic pulmonary vasoconstriction in perinatal lamb)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

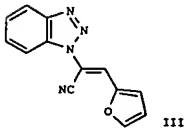
L4 ANSWER 38 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:119110 CAPLUS
DOCUMENT NUMBER: 137:152210
TITLE: Synthesis and antimycobacterial activity of 3-aryl-, 3-cyclohexyl- and 3-heteroaryl-substituted-2-(1H(2H)-benzotriazol-1(2)-yl)prop-2-enenitriles, prop-2-enamides and propenoic acids. II
AUTHOR(S): Sanna, Paolo; Carta, Antonio; Gherardini, Laura; Rahbar Nikookar, Mohammad Esmail
CORPORATE SOURCE: Dipartimento Farmaco-Chimico-Tossicologico, Universita degli Studi, Sassari, 07100, Italy
SOURCE: Farmaco (2002), 57(1), 79-87
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



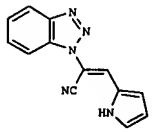
I



II



III

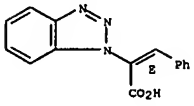


IV

AB A series of 32 3-aryl-, 3-cyclohexyl-, and 3-heteroaryl-substituted-2-(1H(2H)-benzotriazol-1(2)-yl)-prop-2-enenitriles, prop-2-enamides and propenoic acids, was synthesized as a part of our research in the antitubercular field, according to an international program with the Tuberculosis Antimicrobial Acquisition and Coordinating Facility (TAACF). This work reports the preparation and anal. and spectroscopic characterization (MS, UV, IR, 1H NMR) of all compds. synthesized. Among these only a few compds. [I, II, III, IV, and E-2-(1H-benzotriazol-1-yl)-3-(3,4-methylenedioxyphenyl)prop-2-enenitrile] were found to be endowed with

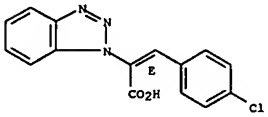
L4 ANSWER 38 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
modest growth inhibition of Mycobacterium tuberculosis. However, the obtained results allowed to acquire interesting structure-activity relationships.
IT 445496-72-0P 445496-73-1P 445496-74-2P
445496-75-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and antimycobacterial activity of aryl-, cyclohexyl-, and heteroaryl-substituted (benzotriazolyl)propenenitriles, propenamides, and propenoic acids)
RN 445496-72-0 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 445496-73-1 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-[(4-chlorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

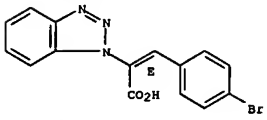
Double bond geometry as shown.



RN 445496-74-2 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-[(4-bromophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

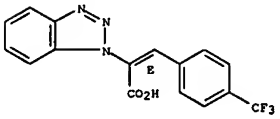
Double bond geometry as shown.

L4 ANSWER 38 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 445496-75-3 CAPLUS
CN 1H-Benzotriazole-1-acetic acid, α-[[4-(trifluoromethyl)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

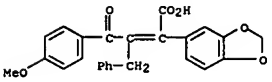
Double bond geometry as shown.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 39 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:86852 CAPLUS
DOCUMENT NUMBER: 136:334989
TITLE: Defective intracellular calcium handling in monocrotaline-induced right ventricular hypertrophy: protective effect of long-term endothelin-a receptor blockade with 2-benzo[1,3]dioxol-5-yl-3-benzyl-4-(4-methoxy-phenyl-)-4-oxobut-2-enoate-sodium (PD 155080)
AUTHOR(S): Brunner, Friedrich; Wolkart, Gerald; Haleen, Stephen
CORPORATE SOURCE: Institut fur Pharmakologie und Toxikologie, Universitat Graz, Graz, Austria
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2002), 300(2), 442-449
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors studied the effect of long-term treatment with the oral endothelin (ET) ETA antagonist 2-benzo[1,3]dioxol-5-yl-3-benzyl-4-(4-methoxy-phenyl-)-4-oxobut-2-enoate-sodium (PD 155080; PD) on right ventricular intracellular Ca (Ca2+i) handling and cardiac and pulmonary artery function in control rats and rats with monocrotaline (MCT)-induced right-heart hypertrophy. Rats were given an i.p. injection of either saline (controls; n = 9) or MCT (50 mg/kg; n = 12), resulting in pulmonary
hypertension-induced myocardial hypertrophy, or MCT followed by the daily administration of PD (50 mg/kg) for 9 wk (n = 9). After 9 wk, right ventricular pressure was measured, and the hearts were removed and perfused in vitro. Right ventricular function and Ca2+i transients were recorded simultaneously on a beat-to-beat basis using aequorin. Surviving
animals in the MCT group (58%) developed significant hypertrophy and had 2-fold higher right ventricular pressure and a prolonged duration of isovolumetric contraction that correlated with a similar prolongation of the Ca2+i transient, indicating a reduced rate of Ca2+ sequestration in hypertrophy. In the PD group, all animals survived, and right ventricular
pressure, diastolic relaxation, Ca2+ transport kinetics, and peak systolic
and end-diastolic wall stress were all normalized; and pulmonary artery endothelial function was partly restored. These results demonstrate for the 1st time that long-term ETA receptor antagonism normalizes myocardial cytosolic Ca2+ modulation, which may contribute to the antihypertrophic and cardioprotective effect of ETA receptor therapy in this model.
IT 162412-71-7, PD 155080
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ETA receptor blockade with PD 155080 and myocardial Ca2+ handling)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 39 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

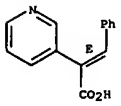


● Na

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 40 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:62733 CAPLUS
DOCUMENT NUMBER: 136:309496
TITLE: Hydrogen bonding networks in E- or Z-2-(3'-pyridyl)-3-phenylpropenoic (α-pyridylcinnamic) acid assemblies - a molecular modeling study
AUTHOR(S): Jojart, Balazs; Palinko, Istvan
CORPORATE SOURCE: Dep. Org. Chem., University Szeged, Szeged, 6720, Hung.
SOURCE: Journal of Molecular Modeling [online computer file] (2001), 7(11), 408-412
CODEN: JMMOFK; ISSN: 0948-5023
URL: http://link.springer.de/link/service/journals/008 94/papers/1007011/10070408.pdf
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
AB The aggregation properties of the stereoisomeric 2-(3-pyridyl)-3-phenylpropenoic acids (PY3E, PY3Z, α-pyridylcinnamic acids) were studied by the PM3 semiempirical quantum chemical method. Calcns. revealed that (aromatic) C-H...N hydrogen bonds made possible the attachment of dimer units. Thus, virtually infinite chains can be built out of PY3E and PY3Z. Three different energy minimized structures were identified: (i) zig-zag, (ii) ladder and (iii) helical configurations.
IT 141694-17-9 233765-13-4
RL: PRP (Properties)
(MO study of infinite chain structures of α-pyridylcinnamic acid isomers)
RN 141694-17-9 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

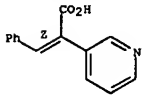
Double bond geometry as shown.



RN 233765-13-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 40 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

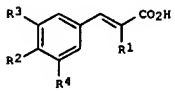


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 41 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:868445 CAPLUS
DOCUMENT NUMBER: 136:5802
TITLE: Preparation of cinnamic acids as fatty acid synthase inhibitors
INVENTOR(S): Leber, Jack Dale; Christensen, Siegfried Benjamin, IV; Daines, Robert A.; Li, Mei; Weinstock, Joseph; Head, Martha S.
PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090099	A1	20011129	WO 2001-US16866	20010524
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001074940	A5	20011203	AU 2001-74940	20010524
EP 1299376	A1	20030409	EP 2001-941601	20010524
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003534340	T	20031118	JP 2001-586286	20010524
US 2003220392	A1	20031127	US 2002-296653	20021125
PRIORITY APPLN. INFO.:			US 2000-206912P	P 20000524
			WO 2001-US16866	W 20010524

OTHER SOURCE(S): MARPAT 136:5802
GI

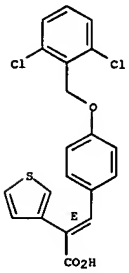


I

AB The title compds. [I; R1 = H, alkyl, aralkyl, etc.; R2 = H, O(CH2)m(hetero)aryl, NR5(CH2)m(hetero)aryl, etc.; R3 = H, halo, OMe, etc.; R4 = H, halo, OMe, Me; R5 = H, alkyl, alkylaryl, etc.; m = 0-3], useful as inhibitors of the fatty acid synthase FabH (no data), were prepared

L4 ANSWER 41 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
multi-step synthesis of (E)-I [R1 = 6-chloropiperonyl; R2, R4 = H; R3 = 2,6-dichlorobenzyloxy] was given.
IT 328064-23-9P 376600-14-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cinnamic acids as fatty acid synthase inhibitors)
RN 328064-23-9 CAPLUS
CN 3-Thiopheneacetic acid, α-[[4-[(2,6-dichlorophenyl)methoxy]phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

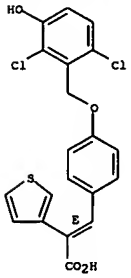
Double bond geometry as shown.



RN 376600-14-5 CAPLUS
CN 3-Thiopheneacetic acid, α-[[4-[(2,6-dichloro-3-hydroxyphenyl)methoxy]phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

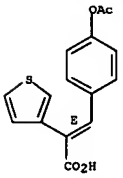
Double bond geometry as shown.

L4 ANSWER 41 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



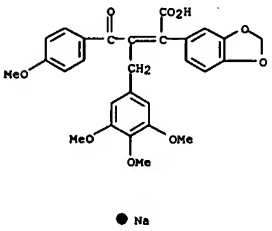
IT 376601-39-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cinnamic acids as fatty acid synthase inhibitors)
RN 376601-39-7 CAPLUS
CN 3-Thiopheneacetic acid, α-[[4-(acetyloxy)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 42 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

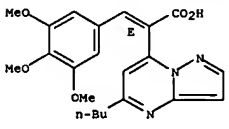
L4 ANSWER 42 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:643955 CAPLUS
DOCUMENT NUMBER: 135:327738
TITLE: Role for endothelin-1-induced superoxide and peroxynitrite production in rebound pulmonary hypertension associated with inhaled nitric oxide therapy
AUTHOR(S): Wedgwood, Stephen; McMullan, D. Michael; Bekker, Janine M.; Fineman, Jeffrey R.; Black, Stephen M.
CORPORATE SOURCE: Dep. Pediatrics and Molecular PHarmacology, Northwestern Univ. Med. Sh., Chicago, IL, USA
SOURCE: Circulation Research (2001), 89(4), 357-364
CODEN: CIRUAL; ISSN: 0009-7330
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Our previous studies have demonstrated that inhaled nitric oxide (NO) decreases nitric oxide synthase (NOS) activity in vivo and that this inhibition is associated with rebound pulmonary hypertension upon acute withdrawal of inhaled NO. We have also demonstrated that inhaled NO elevates plasma endothelin-1 (ET-1) levels and that pretreatment with PD156707, an ETA receptor antagonist, blocks the rebound hypertension. The objectives of this study were to further elucidate the role of ET-1 in the rebound pulmonary hypertension upon acute withdrawal of inhaled NO. Inhaled NO (40 ppm) delivered to thirteen 4-wk-old lambs decreased NOS activity by 36.2% in control lambs (P<0.05), whereas NOS activity was preserved in PD156707-treated lambs. When primary cultures of pulmonary artery smooth muscle cells were exposed to ET-1, superoxide production increased by 33% (P<0.05). This increase was blocked by a preincubation with PD156707. Furthermore, cotreatment of cells with ET-1 and NO increased peroxynitrite levels by 26% (P<0.05), whereas preincubation of purified human endothelial nitric oxide synthase (eNOS) protein with peroxynitrite generated a nitrated enzyme with 50% activity relative to control (P<0.05). Western blot anal. of peripheral lung exts. obtained after 24 h of inhaled NO revealed a 90% reduction in 3-nitrotyrosine residues (P<0.05) in PD156707-treated lambs. The nitration of eNOS was also reduced by 40% in PD156707-treated lambs (P<0.05). These data suggest that the reduction of NOS activity associated with inhaled NO therapy may involve ETA receptor-mediated superoxide production ETA receptor antagonists may prevent rebound pulmonary hypertension by protecting endogenous eNOS activity during inhaled NO therapy.
IT 162412-70-6, PD156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin-1 induced superoxide and peroxynitrite production in rebound pulmonary hypertension upon acute withdrawal of inhaled nitric oxide)
RN 162412-70-6 CAPLUS

L4 ANSWER 43 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:568349 CAPLUS
DOCUMENT NUMBER: 135:157678
TITLE: Intestinal membrane permeability-enhancing agents containing acidic polymers for acidic drugs, and method for improving intestinal membrane permeability of acidic drugs
INVENTOR(S): Terao, Toshimitsu; Matsuda, Kenji
PATENT ASSIGNEE(S): Ohtsuka Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001213805	A	20010807	JP 2000-26335	20000203
PRIORITY APPLN. INFO.:			JP 2000-26335	20000203

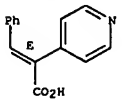
AB The invention relates to an agent for improving intestinal membrane permeability of an acidic drug, wherein the agent is an acidic polymer, especially methacrylic acid-methacrylate ester copolymer. Tablets were prepared from furosemide 20, methacrylic acid-Me methacrylate copolymer (Eudragit L-100-55) 200, hydroxypropyl cellulose 87, lactose 44, and magnesium stearate 1.5 g.
IT 251364-02-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(acidic polymers as intestinal membrane permeability-enhancing agents for acidic drugs)
RN 251364-02-0 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(3,4,5-trimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



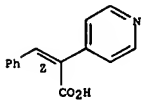
L4 ANSWER 44 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:506468 CAPLUS
DOCUMENT NUMBER: 135:241756
TITLE: Structural motifs in α-pyridyl- and α-furylcinnamic acid assemblies - a molecular modeling study
AUTHOR(S): Palinko, I.; Kortvelyesi, T.
CORPORATE SOURCE: Department of Organic Chemistry, University of Szeged, Szeged, H-6720, Hung.
SOURCE: International Journal of Quantum Chemistry (2001), 84(2), 269-275
CODEN: IJQCB2; ISSN: 0020-7608
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The aggregation properties of stereoisomeric 2-(3'-furyl)-3-phenylpropenoic acids (FU3E, FU3Z, α-furylcinnamic acids) and 2-(4'-pyridyl)-3-phenylpropenoic acids (PY4E, PY4Z, α-pyridylcinnamic acids) were studied by the PM3 semiempirical quantum chemical method. The (aromatic)C-H···N(O) hydrogen bonds make the attachment of dimer units possible; thus, virtually infinite chains can be built out of FU3Z, PY4E, and PY4Z. The energy-minimized structure had zig-zag configuration. PY4Z dimers allowed the formation of a ribbonlike network; however, the number of structural units could not be increased infinitely. One of the furyl derivs. (FU3E) could not be stabilized either in the ribbon or the chain form; however, (aromatic)CH...π or (aromatic)π...(aromatic)π interactions contribute to the packing pattern of the two dimers.
IT 233765-10-1 233765-15-6 340717-68-2 340717-70-6
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(PM3 mol. modeling study of structural motifs in α-pyridyl- and α-furylcinnamic acid assemblies)
RN 233765-10-1 CAPLUS
CN 4-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



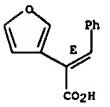
RN 233765-15-6 CAPLUS
CN 4-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

L4 ANSWER 44 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



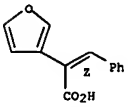
RN 340717-68-2 CAPLUS
CN 3-Furanacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 340717-70-6 CAPLUS
CN 3-Furanacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

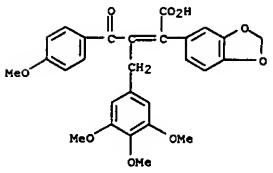
Double bond geometry as shown.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 45 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:276633 CAPLUS
DOCUMENT NUMBER: 135:78493
TITLE: Development of a Scalable Process for CI-1020, A Novel Endothelin Antagonist
AUTHOR(S): Ellis, James E.; Davis, Edward M.; Dozeman, Gary J.; Lenoir, Edward A.; Belmont, Daniel T.; Brower, Phillip L.
CORPORATE SOURCE: Pfizer Global Research and Development, Holland Laboratories Pfizer Inc., Holland, MI, 49424, USA
SOURCE: Organic Process Research & Development (2001), 5(3), 226-233
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The process development of a route for preparing CI-1020 on pilot-plant scale is described in 55% overall yield. Hydrocyanation conditions are described which use acetone cyanohydrin catalyzed by tetramethylammonium hydroxide and which provide the desired ketonitrile intermediate in 85% yield with excellent quality. The penultimate intermediate, a hydroxybutenolide, is prepared in a two-step process using an aldol condensation followed by acid-catalyzed ring closure to give product in 86.8% yield. The active pharmaceutical ingredient (API) is prepared by ring-opening of the hydroxybutenolide with sodium carbonate to provide the sodium salt. The use of ReactIR to monitor the API reaction is described. ReactIR was required to determine an endpoint for the reaction. The use of chromatog. anal. to determine the endpoint was not possible. The API and the penultimate hydroxybutenolide are not separable by chromatog. methods.
IT 162412-70-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(development of a scalable process for a novel endothelin antagonist, CI-1020)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 45 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

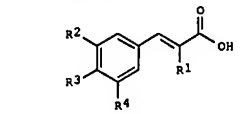
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 46 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:152669 CAPLUS
DOCUMENT NUMBER: 134:193421
TITLE: Preparation of 2'-[heteroaryl(alkyl)]cinnamic acid derivatives as fatty acid synthase inhibitors
INVENTOR(S): Christensen, Siegfried B., IV; Daines, Robert A.; Leber, Jack D.; Pendrak, Israil; Weinstock, Joseph
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

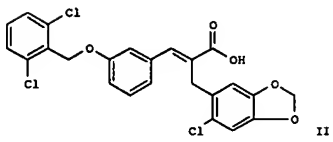
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001014363	A1	20010301	WO 2000-US23019	20000822
W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CZ, DZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1206464	A1	20020522	EP 2000-957669	20000822
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003507468	T	20030225	JP 2001-518450	20000822
US 6498187	B1	20021224	US 2002-49962	20020219
PRIORITY APPLN. INFO.:			US 1999-150212P P	19990823
			WO 2000-US23019 W	20000822

OTHER SOURCE(S): MARPAT 134:193421
GI

L4 ANSWER 46 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



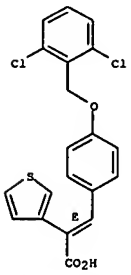
I



II

AB Title compds. (I) [wherein R1 = H, alkyl, (hetero)arylalkyl, (hetero)aryl, or (alkyl)cycloalkyl; R2 = H, O(CH2)mAr, NR5(CH2)mAr, NR6COAr, NR6SO2Ar with proviso; R3 = H, halo, OMe, Me, O(CH2)mAr, NR5(CH2)mAr, NR6COAr, or NR6SO2Ar with proviso; R4 = H, halo, OMe, and Me; R5 = H, alkyl, alkyl(hetero)aryl, acyl, or COAr; R6 = H, alkyl, alkyl(hetero)aryl; Ar = (hetero)aryl; m = 0-3} were prepared as inhibitors of the fatty acid synthase, 3-ketoacyl-ACP synthase (Fab H), for use as a new class of antibiotics. For example, II was formed by coupling 3-(2,6-dichlorobenzyloxy)benzaldehyde with 2-(6-chloropiperonyl)malonic acid monoethyl ester (preparation of starting materials given) in the presence of piperidine and glacial AcOH (67%), followed by deesterification (81%). I are active against a wide range of organisms, including both Gram-neg. organisms, e.g. Escherichia coli and Klebsiella pneumoniae, and Gram-pos. organisms, e.g. Staphylococcus aureus, Streptococcus pneunomiae, Enterococcus faecalis, and Enterococcus faecium, including isolates resistant to existing antibiotics (no data).
IT 328064-23-9P, (E)-4-(2,6-Dichlorobenzyloxy)-2'-(3-thienyl)cinnamic acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of 2'-[heteroaryl(alkyl)]cinnamic acid Fab H inhibitors by coupling benzaldehydes with malonates or acetic acid derivs.)
RN 328064-23-9 CAPLUS
CN 3-Thiopheneacetic acid, α-[[4-[(2,6-dichlorophenyl)methoxy]phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

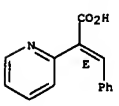
L4 ANSWER 46 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 47 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:45537 CAPLUS
DOCUMENT NUMBER: 134:366557
TITLE: Intramolecular hydrogen bonding in α-phenylcinnamic acids and their heteroatom-containing derivatives studied by ab initio quantum chemical methods
AUTHOR(S): Kortvelyesi, T.; Kukovecz, A.; Lovas, S.; Palinko, I.
CORPORATE SOURCE: Department of Physical Chemistry, University of Szeged, Szeged, H-6720, Hung.
SOURCE: THEOCHEM (2001), 535, 139-149
CODEN: THEODJ; ISSN: 0166-1280
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Intramol. hydrogen bonding interactions were searched for in conformers of isolated α-phenyl-, α-pyridyl- and α-furylcinnamic acid stereoisomers. The conformers were obtained by ab initio (HF/3-21G//HF/3-21G and HF/6-31G(d,p)//HF/6-31G(d,p)) quantum chemical methods using initial geometries corresponding to the global min. determined at the level of semi-empirical quantum chemical calcns. The most common intramol. hydrogen bond was of C-H···O type. In certain conformers of α-(2-pyridyl)cinnamic acids, O-H···Npyridyl and α-(2-furyl)cinnamic acids, O-H···Ofuryl interactions were also found. In most cases, at the level of HF/3-21G calcns., these conformers were more stable than those lacking these close contacts. When the larger basis set was applied the extra stabilizing effect disappeared, nevertheless, these geometries still represented min. structures.
IT 24864-32-2, 2-Pyridineacetic acid, α-(phenylmethylene)-, (E)- 57200-20-1, 2-Furanacetic acid, α-(phenylmethylene)-, (Z)- 61860-38-6, 2-Pyridineacetic acid, α-(phenylmethylene)-, (Z)- 141694-17-9, 3-Pyridineacetic acid, α-(phenylmethylene)-, (E)- 233765-10-1, 4-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- 233765-13-4, 3-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- 233765-15-6, 4-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- 340717-66-0 340717-68-2 340717-70-6
RL: PRP (Properties)
(intramol. hydrogen bonding in α-phenylcinnamic acids and heteroatom-containing derivs. studied by ab initio)
RN 24864-32-2 CAPLUS
CN 2-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

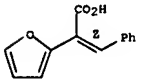
Double bond geometry as shown.



L4 ANSWER 47 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

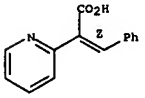
RN 57200-20-1 CAPLUS
CN 2-Furanacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



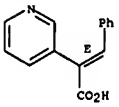
RN 61860-38-6 CAPLUS
CN 2-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 141694-17-9 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

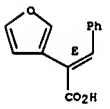


RN 233765-10-1 CAPLUS
CN 4-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

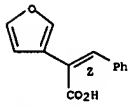
L4 ANSWER 47 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 3-Furanacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



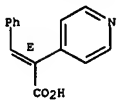
RN 340717-70-6 CAPLUS
CN 3-Furanacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



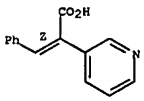
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 47 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



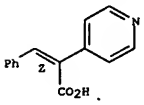
RN 233765-13-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



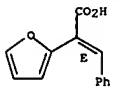
RN 233765-15-6 CAPLUS
CN 4-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 340717-66-0 CAPLUS
CN 2-Furanacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

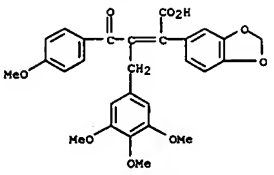
Double bond geometry as shown.



RN 340717-68-2 CAPLUS

L4 ANSWER 48 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:863245 CAPLUS
DOCUMENT NUMBER: 134:247091
TITLE: Effect of endothelin antagonists, including the novel ETA receptor antagonist LBL 031, on endothelin-1 and lipopolysaccharide-induced microvascular leakage in rat airways
AUTHOR(S): Hele, Dave J.; Birrell, Mark A.; Webber, Stephen E.; Foster, Martyn L.; Belvisi, Maria G.
CORPORATE SOURCE: Respiratory Pharmacology Group, Cardiothoracic Surgery, Imperial College School of Medicine, at the National Heart and Lung Institute, London, SW3 6LY, UK
SOURCE: British Journal of Pharmacology (2000), 131(6), 1129-1134
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1 The effect of the novel ETA receptor antagonist LBL 031 and other selective and mixed endothelin receptor antagonists on endothelin-1 (ET-1)-induced and lipopolysaccharide (LPS)-induced microvascular leakage was assessed in rat airways. 2 I.v. administered ET-1 (1 nmole kg-1) or LPS (30 mg kg-1) caused a significant increase in microvascular leakage in rat airways when compared to vehicle-treated animals. 3 Pre-treatment with the selective ETA receptor antagonists, LBL 031 or PD 156707, or the mixed ETA/B receptor antagonist, bosentan (each at 30 mg kg-1), reduced ET-1-induced leakage to baseline levels. ET-1-induced leakage was not reduced by pre-treatment with the ETB selective antagonist BQ 788 (3 mg kg-1). 4 Pre-treatment with the selective ETA receptor antagonist, LBL 031 (0.1 mg kg-1) or PD 156707 (10 mg kg-1), or the mixed ETA/B receptor antagonist, bosentan (30 mg kg-1), reduced LPS-induced leakage by 54, 48 and 59% resp. LPS-induced leakage was not affected by pre-treatment with the ETB selective antagonist BQ 788 (3 mg kg-1). 5 The data suggests that ET-1-induced microvascular leakage in the rat airway is ETA receptor mediated and that part of the increase induced by LPS may be due to the actions of ET-1. Therefore, a potent ETA receptor selective antagonist, such as LBL 031, may provide a suitable treatment for inflammatory diseases of the airways, especially those involving LPS and having an exudative phase, such as the septic shock-induced adult respiratory distress syndrome.
IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effect of endothelin antagonists, including the novel ETA receptor antagonist LBL 031, on endothelin-1 and lipopolysaccharide-induced microvascular leakage in rat airways)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

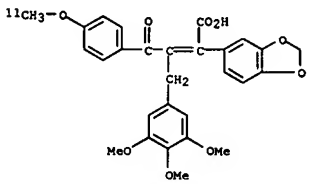
L4 ANSWER 48 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 49 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:776045 CAPLUS
DOCUMENT NUMBER: 134:46705
TITLE: Syntheses of the first endothelin-A- and -B-selective radioligands for positron emission tomography
AUTHOR(S): Johnstrom, Peter; Aigbirhio, Franklin I.; Clark, John C.; Downey, Steve P. M. J.; Pickard, John D.; Davenport, Anthony P.
CORPORATE SOURCE: Clinical Pharmacology Unit, Addenbrooke's Hospital, University of Cambridge, Cambridge, UK
SOURCE: Journal of Cardiovascular Pharmacology (2000), 36(5, Suppl. 1), S58-S60
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have synthesized two potential positron emission tomog. (PET) radioligands for the endothelin (ET) receptor. [11C]-PD156707 was produced by O-methylation of PD169390 using [11C]iodomethane. Radiochem. conversions of the order of 74 ± 3.2% (n = 8) were obtained. The radiochem. purity of the isolated [11C]-PD156707 was 99% and the specific activity was 538 mCi/μmol. [18F]-BQ3020 was produced from [18F]fluoride in a total radiochem. yield of 2.7 ± 0.4% (n = 10) in 238 ± 5 min. The radiochem. purity was 95% and specific activities of the order of 670-930 mCi/μmol were obtained.
IT 313071-42-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of endothelin-A- and -B-selective radioligands for positron emission tomog.)
RN 313071-42-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-[4-(methoxy-11C)phenyl]-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX
NAME)

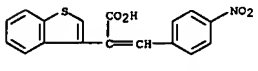


● Na

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

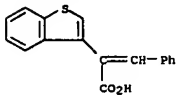
L4 ANSWER 49 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 50 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:708008 CAPLUS
DOCUMENT NUMBER: 134:17374
TITLE: Synthesis of thiopyrone and pyrone derivatives by photocyclization reaction of 3-aryl-2-([1]benzothien-3-yl)propenoic acids
AUTHOR(S): Sasaki, Kenji; Satoh, Yasuyoshi; Hirota, Takashi; Nakayama, Taiji; Tominaga, Yoshinori; Castle, Raymond N.
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Okayama University, Okayama, 700-8530, Japan
SOURCE: Journal of Heterocyclic Chemistry (2000), 37(4), 959-967
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:17374
AB Naphtho[1,2-b][1]benzothiophene-6-carboxylic acids, 6H-benzo[b]naphtho[2,3-d]thiopyran-6-ones and 6H-benzo[b]naphtho[2,3-d]pyran-6-ones were synthesized in one step by the photocyclization reaction of 3-aryl-2-([1]benzothien-3-yl)propenoic acids. The photocyclization reaction did not occur when the 3-aryl group contained the electron-withdrawing nitro group. The assignment of the 1H and 13C NMR spectra of 6H-benzo[b]naphtho[2,3-d]thiopyran-6-one and 6H-benzo[b]naphtho[2,3-d]pyran-6-one by two-dimensional NMR methods is described. The difference between the chemical shift values of H12 for these two compds. is attributed to different mol. geometries.
IT 310462-44-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 310462-44-3 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, α-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

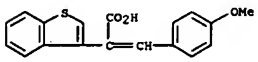


IT 183018-47-5P 310462-41-0P 310462-42-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of naphthobenzothiophenecarboxylates, benzonaphthothiopyranones and benzonaphthopyranones by cyclization of (aryl)benzothienylpropenoates)
RN 183018-47-5 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)

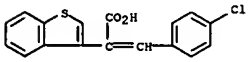
L4 ANSWER 50 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



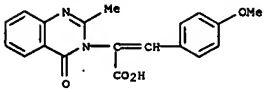
RN 310462-41-0 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



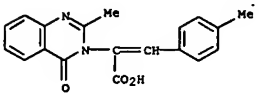
RN 310462-42-1 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, α-[(4-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)



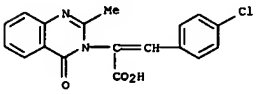
L4 ANSWER 51 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



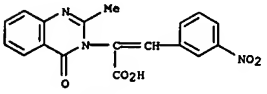
RN 286367-36-0 CAPLUS
CN 3(4H)-Quinazolineacetic acid, 2-methyl-α-[(4-methylphenyl)methylene]-4-oxo- (9CI) (CA INDEX NAME)



RN 286367-37-1 CAPLUS
CN 3(4H)-Quinazolineacetic acid, α-[(4-chlorophenyl)methylene]-2-methyl-4-oxo- (9CI) (CA INDEX NAME)

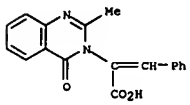


RN 286367-38-2 CAPLUS
CN 3(4H)-Quinazolineacetic acid, 2-methyl-α-[(3-nitrophenyl)methylene]-4-oxo- (9CI) (CA INDEX NAME)



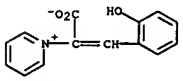
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 51 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:358557 CAPLUS
DOCUMENT NUMBER: 133:135295
TITLE: Azlactones in heterocyclic synthesis: Part III - A novel method for the synthesis of 2-methyl-3-styryl-4(3H)-quinazolinone and 3-arylidene-4-benzoyl-1,4-benzodiazepine-2,5-dione derivatives
AUTHOR(S): Subhashini, N. J. P.; Hanumanthu, P.
CORPORATE SOURCE: Department of Chemistry, Osmania University, Hyderabad, 500 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2000), 39B(3), 198-201
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Condensation of 2-methyl-and 2-phenyl-4-arylidene-2-oxazolin-5-ones (azlactones) with o-aminobenzamide in acetic acid results in two diverse heterocyclic compds., α-[2-methyl-4(3H)-quinazolinon-3-yl]cinnamic acid and 3-arylidene-4-benzoyl-1,4-benzodiazepine-2,5-diones, resp. Structures of these compds. have been established based on their spectral data and elemental analyses.
IT 286367-34-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methylstyrylquinazolinone and arylidenebenzoylbenzodiazepine dione derivs.)
RN 286367-34-8 CAPLUS
CN 3(4H)-Quinazolineacetic acid, 2-methyl-4-oxo-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



IT 286367-35-9P 286367-36-0P 286367-37-1P
286367-38-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of methylstyrylquinazolinone and arylidenebenzoylbenzodiazepine dione derivs.)
RN 286367-35-9 CAPLUS
CN 3(4H)-Quinazolineacetic acid, α-[(4-methoxyphenyl)methylene]-2-methyl-4-oxo- (9CI) (CA INDEX NAME)

L4 ANSWER 52 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:337684 CAPLUS
DOCUMENT NUMBER: 133:120255
TITLE: Synthesis of hetarylpyridinium salts and fused 3-aminopyrid-2-ones
AUTHOR(S): Rehwald, Matthias; Bellmann, Peter; Jeschke, Torsten; Gewald, Karl
CORPORATE SOURCE: Degussa-Huls, Werk Radebeul, Radebeul, Germany
SOURCE: Journal fuer Praktische Chemie (Weinheim, Germany) (2000), 342(4), 371-378
CODEN: JPCHF4; ISSN: 1436-9966
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 133:120255
AB 1-(3-Coumaryl)pyridinium salts and -tetrahydrothiophenium salts were synthesized from 2-acylphenyl haloacetates. 2-Chloro-N-(3,4-dimethoxyphenyl)acetamide and substituted 2-chloro-N-thien-2-ylacetamides react with AcCl and pyridine to yield the quinolinyl- and (thieno[2,3-b]pyridin-5-yl)pyridinium salts (I). Fused thieno[2,3-b]pyridinones were formed from N-(chloroacetyl)-2-aminothiophene-3-carbonitriles with pyridine via Thorpe-Ziegler cyclization, followed by cyclodehydrogenation. In presence of pyridine, alkyl 2-[(chloroacetyl)amino]benzoates yield 3-(1-pyridinio)quinolin-4-olates (II). Zincke-cleavage of I and II with N2H4.H2O leads to fused 3-aminopyridin-2-ones and 3-amino-4-hydroxyquinolin-2-ones (III), resp. Oxazoloquinolines were synthesized from III with Ac2O.
IT 285138-52-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of hetarylpyridinium salts and fused aminopyridones)
RN 285138-52-5 CAPLUS
CN Pyridinium, 1-[1-carboxy-2-(2-hydroxyphenyl)ethenyl]-, inner salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

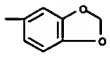
L4 ANSWER 53 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:259979 CAPLUS
DOCUMENT NUMBER: 132:288794
TITLE: Sympathetic nervous system activity-reducing agents for treatment of disease- or age-related weight loss and for enhancement of exercise performance
INVENTOR(S): Anker, Stefan Dietmar; Coats, Andrew Justin Stewart
PATENT ASSIGNEE(S): Imperial College Innovations Limited, UK
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000021509	A2	20000420	WO 1999-GB3302	19991015
WO 2000021509	A3	20001109		
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1121111	A2	20010808	EP 1999-947762	19991015
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002527378	T	20020827	JP 2000-575485	19991015
PRIORITY APPLN. INFO.:			GB 1998-22458	A 19981015
			GB 1998-22459	A 19981015
			GB 1999-17181	A 19990723
			WO 1999-GB3302	W 19991015

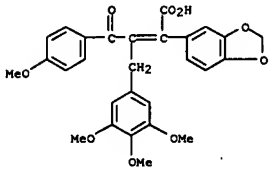
AB A method of treating weight loss due to underlying disease in a patient, the method comprising administering to the patient an effective amount of an agent which reduces sympathetic nervous system activity. A method of treating weight loss due to underlying disease in a patient, the method comprising administering to the patient an effective amount of any one or more of the following: a compound which inhibits the effect of aldosterone such as an aldosterone antagonist; a chymase inhibitor; a cathepsin B inhibitor; a β receptor blocker; an imidazoline receptor antagonist; a centrally acting α receptor antagonist; a peripherally acting α receptor antagonist; a ganglion blocking agent; a drug that has an effect on cardiovascular reflexes and thereby reduces SNS activity such as an opiate; scopolamine; an endothelin receptor antagonist; and a xanthine oxidase inhibitor. The methods are particularly useful in treating cardiac cachexia. The sympathetic nervous system activity-reducing agents may also be used to treat weight loss due to aging and to enhance exercise performance.
IT 162412-70-6, PD 156707 204326-22-7, PD 164333

L4 ANSWER 53 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B



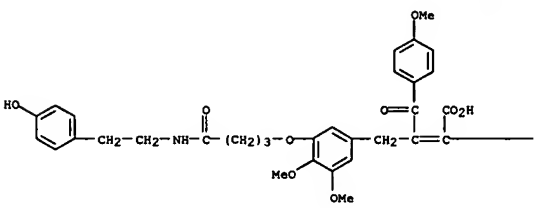
L4 ANSWER 53 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (sympathetic nervous system activity-reducing agents for treatment of disease- or age-related wt. loss and for enhancement of exercise performance)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

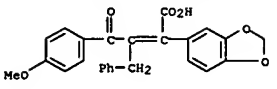
RN 204326-22-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-[4-[[2-(4-hydroxyphenyl)ethyl]amino]-4-oxobutoxy]-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

PAGE 1-A



L4 ANSWER 54 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:8345 CAPLUS
DOCUMENT NUMBER: 132:164477
TITLE: Effects on hemodynamics by selective endothelin ETB receptor and combined endothelin ETA/ETB receptor antagonism during endotoxin shock
AUTHOR(S): Wanecek, M.; Oldner, A.; Sundin, P.; Alving, K.; Weitzberg, E.; Rudehill, A.
CORPORATE SOURCE: Department of Anaesthesiology and Intensive Care, Karolinska Hospital, Stockholm, S-171 76, Swed.
SOURCE: European Journal of Pharmacology (1999), 386(2/3), 235-245
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The endothelin system is highly activated during endotoxin and septic shock. To investigate this matter the selective non-peptide endothelin ETB receptor antagonist A-192621 ([2R-(2α,3β,4α)]-4-(1,3-benzodioxol-5-yl)-1-[[2-(2,6-diethylphenyl)amino]-2-oxoethyl]-2-(4-propoxyphenyl)-3-pyrrolidinecarboxylic acid) was administered alone and in combination with the selective non-peptide endothelin ETA receptor antagonist PD 155080 (sodium 2-benzo[1,3]dioxol-5-yl-3-benzyl-4-(4-methoxyphenyl)-4-oxobut-2-enoate)during established porcine endotoxin shock. Cardiopulmonary vascular function, metabolic parameters and plasma endothelin-1-like immunoreactivity levels were compared to a control group only receiving endotoxin. Administration of A-192621 alone resulted in cardiovascular collapse and death, whereas combining A-192621 with PD 155080 abolished endotoxin induced pulmonary hypertension, enhanced cardiac performance and improved systemic oxygen delivery and acid-base balance. The beneficial effects of mixed endothelin ETA/ETB receptor antagonisms on the pulmonary and cardiovascular systems may result from blockage of constrictive endothelin receptors in the pulmonary circulation, reduced afterload and a direct inotropic effect. Possible mechanisms for the devastating effects by selective endothelin ETB receptor antagonism include increased endothelin ETA receptor-mediated vasoconstriction due to lack of endothelin ETB receptor-mediated vasodilation and decreased endothelin clearance from endothelin ETB receptor blockade. In conclusion, selective endothelin ETB receptor antagonism is deleterious, whereas combined endothelin ETA and ETB receptor antagonism has favorable effects on hemodynamics, suggesting participation of the endothelin system in cardiopulmonary dysfunction during endotoxin shock.
IT 162412-71-7, PD 155080
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (effects on hemodynamics by selective endothelin ETB receptor and combined endothelin ETA/ETB receptor antagonism during endotoxin shock)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 54 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

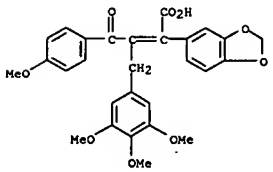
L4 ANSWER 55 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 55 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:812692 CAPLUS
DOCUMENT NUMBER: 132:166140
TITLE: Synthetic approaches to endothelin receptor antagonists in clinical development
AUTHOR(S): Clark, William M.
CORPORATE SOURCE: Synthetic Chemistry Department, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406, USA
SOURCE: Current Opinion in Drug Discovery & Development (1999), 2(6), 565-577
CODEN: CODDFF; ISSN: 1367-6733
PUBLISHER: Current Drugs Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB The increasing structural and stereochem. complexity of new drug candidates continues to pose numerous synthetic challenges for pharmaceutical process development. Often the implementation of new methodologies, and/or the novel utilization of existing methodologies becomes an essential aspect of developing cost-effective and practical syntheses for new chemotherapeutics. An excellent case in point, and highlighted in this review with 29 refs., are the novel synthetic processes developed for some of the leading endothelin receptor antagonists currently in clin. development.

IT 162412-70-6P, PD-156707
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(synthetic approaches to endothelin receptor antagonists in clin. development)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



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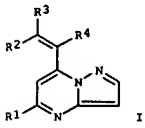
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:753238 CAPLUS
DOCUMENT NUMBER: 132:12322
TITLE: Preparation of pyrazolo[1,5-a]pyrimidine derivatives as nitrogen monoxide synthase inhibitors
INVENTOR(S): Okamura, Takashi; Shoji, Yasuo; Shibutani, Tadao; Yasuda, Tsuneo; Iwamoto, Takeshi
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Factory, Inc., Japan
SOURCE: PCT Int. Appl., 109 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9959998	A1	19991125	WO 1999-JP2572	19990517
W: AU, CA, CN, JP, KR, NO, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2331468	A1	19991125	CA 1999-2331468	19990517
CA 2331468	C	19991125		
AU 9937320	A	19991206	AU 1999-37320	19990517
AU 751337	B2	20020815		
EP 1081149	A1	20010307	EP 1999-919634	19990517
EP 1081149	B1	20030402		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AT 236166	T	20030415	AT 1999-919634	19990517
CN 1117093	B	20030806	CN 1999-805673	19990517
NO 2000005820	A	20001117	NO 2000-5820	20001117
NO 317303	B1	20041004		
US 6372749	B1	20020416	US 2000-700764	20001120
PRIORITY APPLN. INFO.:			JP 1998-136960 A	19980519
			WO 1999-JP2572 W	19990517

OTHER SOURCE(S): MARPAT 132:12322
GI



I

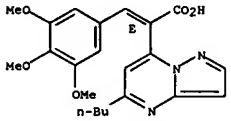
AB Pyrazolo[1,5-a]pyrimidine derivs. represented by general formula [I; R1 = lower alkyl, Ph, thienyl; one of R2 and R3 = H and the other = naphthyl, furyl, pyridyl, styryl, phenylethynyl, (un)substituted Ph; R4 = H, lower alkylthio, lower alkylsulfinyl, lower alkylsulfonyl, CO2H, lower alkoxycarbonyl, et.], which have pharmacol. effects including analgesic effect and nitrogen monoxide synthase inhibitory effect and are useful as

L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
analgesic agents and remedies and preventives for sepsis, endotoxin shock,
chronic rheumatoid arthritis, etc., are prepd. Thus, 1.0 g di-Et (5-n-butylpyrazolo[1,5-a]pyrimidin-7-yl)methylphosphonate and 0.66 g 3,4,5-trimethoxybenzaldehyde were dissolved in 5.0 mL ethanol, cooled to 0°, treated with 3.8 mL 5% aq. NaOH, and stirred at 0° for 1 h to give the title compd. (I; R1 = n-Bu, R2 = R4 = H, R3 = 3,4,5-trimethoxyphenyl) (II). In an analgesic assay against pressure-stimulated pain, II in vivo showed 47.8% recovery ratio of pain threshold value in the rear sole of rat in 60 min after the treatment with
substance P. Pharmaceutical formulation contg. I were also prepd.

IT 251364-02-0P 251364-03-1P 251364-04-2P
251364-05-3P 251364-06-4P 251364-07-5P
251364-08-6P 251364-09-7P 251364-11-1P
251364-12-2P 251364-15-5P 251364-16-6P
251364-17-7P 251364-18-8P 251364-19-9P
251364-20-2P 251364-62-2P 251364-63-3P
251364-64-4P 251364-66-6P 251364-70-2P
251364-71-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolo[1,5-a]pyrimidine derivs. as nitrogen monoxide synthase inhibitors and analgesics and for treatment and prevention of endotoxin shock, and chronic rheumatoid arthritis)

RN 251364-02-0 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(3,4,5-trimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

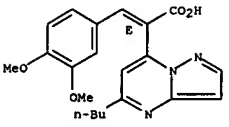
Double bond geometry as shown.



RN 251364-03-1 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(3,4-dimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

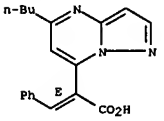
Double bond geometry as shown.

L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



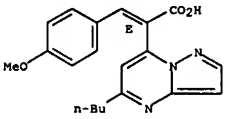
RN 251364-04-2 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 251364-05-3 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(4-methoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

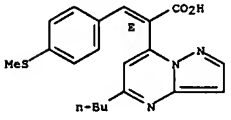
Double bond geometry as shown.



RN 251364-06-4 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(4-(methylthio)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

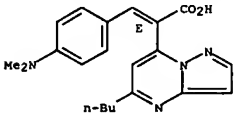
Double bond geometry as shown.

L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



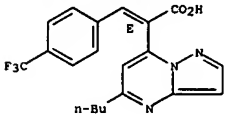
RN 251364-07-5 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[[4-(dimethylamino)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



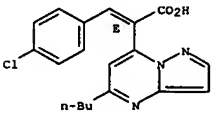
RN 251364-08-6 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[[4-(trifluoromethyl)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 251364-09-7 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(4-chlorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

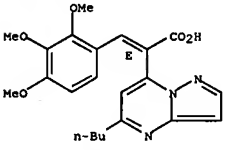
Double bond geometry as shown.



L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

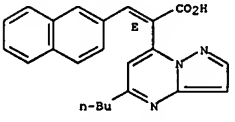
RN 251364-11-1 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(2,3,4-trimethoxyphenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



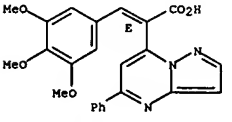
RN 251364-12-2 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-(2-naphthalenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 251364-15-5 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-phenyl-α-[(3,4,5-trimethoxyphenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

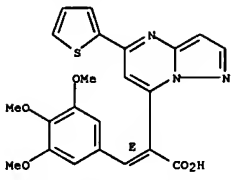
Double bond geometry as shown.



RN 251364-16-6 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-(2-thienyl)-α-[(3,4,5-trimethoxyphenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

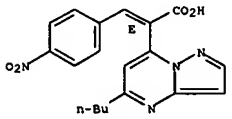
Double bond geometry as shown.

L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



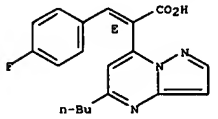
RN 251364-17-7 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(4-nitrophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 251364-18-8 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(4-fluorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

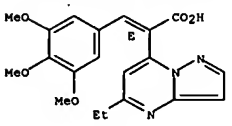
Double bond geometry as shown.



RN 251364-19-9 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, α-([1,1'-biphenyl]-4-ylmethylene)-5-butyl-, (αE)- (9CI) (CA INDEX NAME)

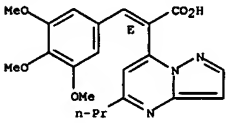
Double bond geometry as shown.

L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



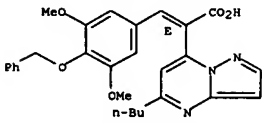
RN 251364-64-4 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-propyl-α-[(3,4,5-trimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



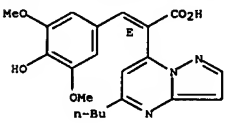
RN 251364-66-6 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[[3,5-dimethoxy-4-(phenylmethoxy)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

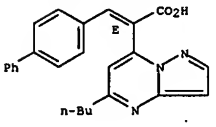


RN 251364-70-2 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(4-hydroxy-3,5-dimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

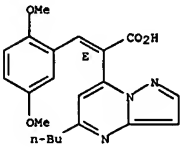


L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



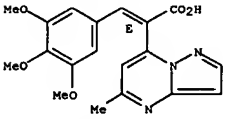
RN 251364-20-2 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(2,5-dimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 251364-62-2 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-methyl-α-[(3,4,5-trimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



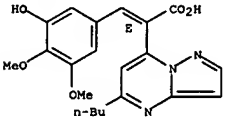
RN 251364-63-3 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-ethyl-α-[(3,4,5-trimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 56 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 251364-71-3 CAPLUS
CN Pyrazolo[1,5-a]pyrimidine-7-acetic acid, 5-butyl-α-[(3-hydroxy-4,5-dimethoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



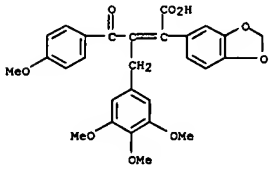
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 57 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:722912 CAPLUS
DOCUMENT NUMBER: 131:317804
TITLE: Methods for treatment of pain by inhibiting endothelin-1 action
INVENTOR(S): Davar, Gudarz
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9956761	A1	19991111	WO 1999-US9732	19990504
W: AU, CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6673832	B1	20040106	US 1998-72428	19980504
AU 9937849	A	19991123	AU 1999-37849	19990504
PRIORITY APPLN. INFO.:			US 1998-72428	A 19980504
			WO 1999-US9732	W 19990504

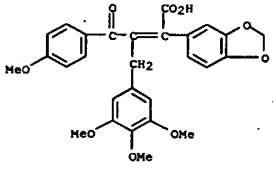
AB A method of determining whether a compound alleviates nerve pain mediated by endothelin-1 (ET-1) involves (i) determining whether the compound has the ability to inhibit a ET-1 action and then (ii) determining whether the compound reduces nerve pain by testing the compound in human patients suffering from pain mediated by the ET-1 action. The invention also includes a method of determining whether a compound alleviates pain caused by nerve injury in human patients by determining the compound ability to inhibit an inflammatory leukocyte response. ET-1 (40-800 μM) applied to rat sciatic nerve in vivo induced direct effect on sensory neurons and pain behavior via a mechanism independent of vasoconstriction of sciatic nerve microvessels. ET-1-induced pain behavior is mediated by ATA subtype of receptor on neurons, as evidenced by using ETA and ETB receptor antagonists, BQ-123 and BQ-788, resp. Therefore, the inhibition of ET-1's vasoconstriction-independent mechanism of causing pain is an effective pain treatment, especially under conditions where ET-1 levels are elevated in a patient, such as metastatic prostate cancer. Furthermore, given that ET-1 acts directly on the sensory neuron ETA receptor, the ETA receptor is an important therapeutic target.
IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

L4 ANSWER 57 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Uses)
(assay for evaluation of endothelin receptor antagonists for treatment vasoconstriction-independent of pain)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

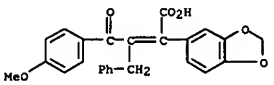
L4 ANSWER 58 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:637955 CAPLUS
DOCUMENT NUMBER: 132:131572
TITLE: PD-156707 Parke-Davis
AUTHOR(S): Hopfner, Robert
CORPORATE SOURCE: Department of Pharmacology College of Medicine, University of Saskatchewan, Saskatoon, SK, S7N 5E5, Can.
SOURCE: Current Opinion in Cardiovascular, Pulmonary & Renal Investigational Drugs (1999), 1(3), 433-442
CODEN: CCPRFX; ISSN: 1464-8482
PUBLISHER: Current Drugs Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 110 refs. PD-156707 is a non-peptide endothelin ETA antagonist which is being investigated by Parke-Davis as a potential treatment for hypertension. An IND has been submitted to the US FDA, seeking permission to begin clin. development. Preclin. studies also indicate efficacy in animal models of congestive heart failure (CHF), pulmonary hypertension and cerebral ischemia. Chronic dosing studies with PD-156707 (40 mg/kg/day) demonstrated a 44% decrease in mean pulmonary arterial pressure (MPAP) and a 23% decrease in the right ventricular hypertrophy index. The activity of PD-156707 is 10-fold more active than Roche's bosentan (qv), and is also effective in the post-infusion treatment of cerebral ischemia caused by the occlusion of the middle cerebral artery.
IT 162412-70-6P, PD-156707
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(development of endothelin ETA receptor antagonist PD-156707 as an antihypertensive drug)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



L4 ANSWER 58 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
REFERENCE COUNT: 110 THERE ARE 110 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 59 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:602838 CAPLUS
DOCUMENT NUMBER: 131:295334
TITLE: Differentiated effects on splanchnic homeostasis by selective and non-selective endothelin receptor antagonism in porcine endotoxaemia
AUTHOR(S): Oldner, Anders; Wanecek, Michael; Weitzberg, Eddie; Sundin, Pierre; Sollevi, Alf; Rubio, Carlos; Hellstrom, Per M.; Alving, Kjell; Rudehill, Anders
CORPORATE SOURCE: Department of Anaesthesiology & Intensive Care, Karolinska Hospital, Stockholm, SE-171 76, Swed.
SOURCE: British Journal of Pharmacology (1999), 127(8), 1793-1804
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Stockton Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The non-selective endothelin (ET) receptor antagonist bosentan has been shown to restore systemic and gut oxygen delivery and reverse intestinal mucosal acidosis in porcine endotoxin shock. To further elucidate the specific role of the ETA as opposed to the ETB receptor and their effects in the splanchnic region, a non-selective (ETMIXra) A-182086 and selective ETA (ETAra) PD155080 and ETB (ETBra) A-192621 receptor antagonists were administered, sep. or simultaneously (ETA+Bra) 2 h after onset of endotoxin shock. These four groups were compared to a control group receiving only endotoxin and vehicle. Thirty-nine pigs were anesthetized and catheterized for measurement of central and regional hemodynamics. A tonometer in the distal ileum was used for measurement of mucosal PCO2. Blood gases and plasma ET-1-LI levels as well as histol. samples from the gut were assessed. Intervention was started 2 h after onset of endotoxemia and the expts. were terminated after 5 h. Endotoxin-induced changes in systemic, gut oxygen delivery and portal hepatic vascular resistance and systemic acidosis were effectively counteracted by both ETA+Bra and ETMIXra. ETAra administration was not effective while ETBra proved to be fatal as all animals in this group died prior to full time of the experiment While both ETA-Bra and ETMIXra improved gut oxygen delivery, only the latter attenuated the profound endotoxin-induced ileal mucosal acidosis. The lethal effect seen from selective ETB receptor antagonism in the current study may be due to increased ETA receptor activity as plasma levels of ET-1 is increased several fold by blocking the ETB receptor and thereby the plasma-ET-1-clearing function. Furthermore, a loss of endothelial ETB receptor vasodilating properties may also have contributed to the lethal course in the ETBra group. The findings in this study suggest that ET is involved in the profound endotoxin-induced disturbances in splanchnic homeostasis in porcine endotoxemia. Furthermore, antagonism of both ETA and ETB receptors is necessary to effectively counteract these changes.
IT 162412-71-7, PD155080
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

L4 ANSWER 59 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Uses)
(differentiated effects on splanchnic homeostasis by selective and non-selective endothelin receptor antagonism in porcine endotoxemia in relation to role of ETA and ETB receptors)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

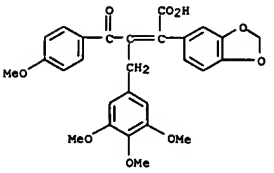


● Na

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 60 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:322907 CAPLUS
DOCUMENT NUMBER: 131:134538
TITLE: Butenolide Endothelin Antagonists with Improved Aqueous Solubility
AUTHOR(S): Patt, William C.; Cheng, Xue-Min; Repine, Joseph T.; Lee, Chet; Reisdorph, Bill R.; Massa, Mark A.; Doherty, Annette M.; Welch, Kathleen M.; Bryant, John W.; Flynn, Michael A.; Walker, Donnelle M.; Schroeder, Richard L.; Haleen, Stephen J.; Keiser, Joan A.
CORPORATE SOURCE: Departments of Chemistry and Vascular and Cardiac Diseases Parke-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (1999), 42(12), 2162-2168
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Continued development around our ETA-selective endothelin (ET) antagonist (CI-1020) (I) has led to the synthesis of analogs with improved aqueous solubility profiles. Poor solubility characteristics displayed by I required a complex buffered formulation in order to conduct iv studies. To overcome the use of specific iv formulations for preclin. studies on addnl. drug candidates, analogs with improved aqueous solubility were desired. Several analogs were prepared with substitution patterns that allowed for the formation of either acid or base addition salts. These derivs. had dramatically improved aqueous solubility In addition, these analogs retained equivalent or improved ETA receptor selectivity and antagonist potency, vs. I, both in vitro and in vivo. One of the compds., which contains as a substituent the sodium salt of a sulfonic acid, has an ETA IC50 0.38 nM, ETA selectivity of 4200-fold, and ETA functional activity of KB 7.8, all of which are similar or superior to those of I. This compound also has vastly superior aqueous solubility and solubility duration superior to that of I and after i.v. infusion displays an improved activity over I in preventing acute hypoxia-induced pulmonary hypertension in rats with an ED50 0.3 μg/kg/h.
IT 162412-70-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(preparation of butenolide endothelin antagonists with improved aqueous solubility)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 60 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

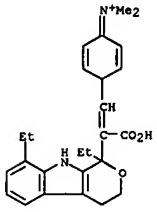
L4 ANSWER 61 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:300958 CAPLUS
DOCUMENT NUMBER: 131:92616
TITLE: Spectrophotometric and spectrofluorimetric determination of etodolac and aceclofenac
AUTHOR(S): El Kousy, N. M.
CORPORATE SOURCE: National Organization for Drug Control and Research, Cairo, Egypt
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (1999), 20(1-2), 185-194
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two simple, sensitive and reproducible spectrophotometric and spectrofluorimetric methods were adopted for the anal. of the anti-inflammatory drugs, etodolac and aceclofenac. The first method was based on the formation of colored complexes between the drugs and p-dimethylaminobenzaldehyde reagent (PDAB) in the presence of sulfuric acid and ferric chloride. Measurement of the absorbances was carried out at 591.5 and 545.5 nm for etodolac and aceclofenac, resp. Regression anal. of Beer's plots showed good correlation in the concentration ranges 10-80 and 8-55 μg ml-1, resp. The second was the spectrofluorimetric method in which samples of etodolac in ethanol showed native fluorescence at λ 345 nm when excitation was at 235 nm and samples of aceclofenac in the phosphate buffer pH 8 showed native fluorescence at λ 355 nm when excitation was at 250 nm. The calibration graph was rectilinear from 96 to 640 ng mL-1 for etodolac and from 2 to 8 μg mL-1 for aceclofenac. The proposed methods were applied successfully for the determination of the 2 drugs in bulk with a mean accuracy of 100.48 and 100.03% in the PDAB method and of 100.61 and 99.88% in the spectrofluorimetric method. Applicability of the proposed methods was examined by analyzing dosage forms of the drugs. Recoveries were 98.77-101.46 and 98.65-102.10% for the 2 methods, resp. and RSD values were 0.6-0.7 and 0.35-1.06%, resp.

IT 229333-81-7
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(spectrophotometric and spectrofluorimetric determination of etodolac and aceclofenac)

RN 229333-81-7 CAPLUS
CN Methanaminium, N-[4-[2-carboxy-2-(1,8-diethyl-1,3,4,9-tetrahydropyrano[3,4-b]indol-1-yl)ethenyl]-2,5-cyclohexadien-1-ylidene]-N-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 61 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

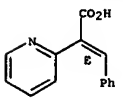
L4 ANSWER 62 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:216054 CAPLUS
DOCUMENT NUMBER: 131:129801
TITLE: Structure and E-Z isomerization of α-pyridylcinnamic acids studied by ab initio and semiempirical methods
AUTHOR(S): Kortvelyesi, T.; Lovas, S.; Murphy, R. F.; Kiss, G.; Palinko, I.
CORPORATE SOURCE: Dep. Physical Chem., Jozsef Attila Univ., Szeged, H-6720, Hung.
SOURCE: Internet Journal of Chemistry [Electronic Publication] (1999), 2, No pp. Given, Article 2
CODEN: IJCHFJ
URL: http://www.ijc.com/articles/1999v2/2/abstract.pdf
PUBLISHER: Internet Journal of Chemistry
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB Cinnamic acids containing a pyridyl group with variously positioned nitrogen in the position α relative to the carboxylic group were studied at the level of semiempirical quantum chemical and ab initio MO methods. Comparison of the total energies or standard enthalpies of formation data in the fully optimized structures of the stereoisomer pairs revealed that their thermodn. stabilities are not dramatically different at the HF/3-21 G(*) level and negligible at the level of semiempirical quantum chemical methods (AM1, MNDO, PM3). Structures computed at ab initio level are reported. The E-Z (and Z-E) isomerization reactions of the neutral mols. in the gas phase are investigated at the semiempirical quantum chemical level of theory (AM1, MNDO and PM3). Reaction and activation enthalpies for the configurational isomerization reaction were computed and the transition-state structures were determined

IT 24864-32-2 61860-38-6 141694-17-9 233765-10-1 233765-13-4 233765-15-6
RL: PRP (Properties)
(structure and E-Z isomerization of α-pyridylcinnamic acids studied by ab initio and semiempirical methods)

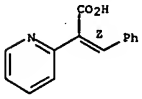
RN 24864-32-2 CAPLUS
CN 2-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



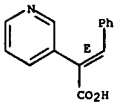
RN 61860-38-6 CAPLUS
CN 2-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

L4 ANSWER 62 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



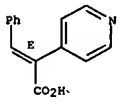
RN 141694-17-9 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



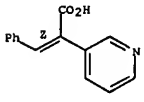
RN 233765-10-1 CAPLUS
CN 4-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 233765-13-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

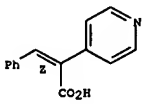
Double bond geometry as shown.



RN 233765-15-6 CAPLUS
CN 4-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

L4 ANSWER 62 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
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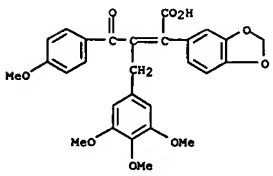
L4 ANSWER 63 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 63 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:195439 CAPLUS
DOCUMENT NUMBER: 131:14403
TITLE: Blockade and reversal of endothelin-induced constriction in pial arteries from human brain
AUTHOR(S): Pierre, Lisa N.; Davenport, Anthony P.
CORPORATE SOURCE: Clinical Pharmacology Unit, University of Cambridge, Cambridge, CB2 2QQ, UK
SOURCE: Stroke (1999), 30(3), 638-643
CODEN: SJCCA7; ISSN: 0039-2499
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Substantial evidence now implicates endothelin (ET) in the pathophysiol. of cerebrovascular disorders such as the delayed vasospasm associated with subarachnoid hemorrhage and ischemic stroke. The authors investigated the ET receptor subtypes mediating vasoconstriction in human pial arteries. ET receptors on human pial and intracerebral arteries were visualized with the use of autoradiog., and the subtypes mediating vasoconstriction were identified by wire myog. ET-1 was more potent than ET-3 as a vasoconstrictor, indicating an ETA-mediated effect. Similarly, the selective ETB agonist sarafotoxin S6c had no effect on contractile action at concns. up to 30 nmol/L. The nonpeptide ETA receptor antagonist PD156707 (3 to 30 nmol/L) caused a parallel rightward shift of the ET-1-induced response, yielding a pA2 of 9.2. Consistent with these results, PD156707 (30 nmol/L) fully reversed an established constriction in pial arteries induced by 1 nmol/L ET-1, while the selective ETB receptor antagonist BQ788 (1 μM) had little effect. The calcium channel blocker nimodipine (0.3 to 3 μM) significantly attenuated the maximum response to ET-1 in a concentration-dependent manner without changing potency. In agreement with the functional data, specific binding of [125I]PD151242 to ETA receptors was localized to the smooth muscle layer of pial and intracerebral blood vessels. In contrast, little or no [125I]BQ3020 binding to ETB receptors was detected. These data indicate an important role for ETA receptors in ET-1-induced constriction of human pial arteries and suggest that ETA receptor antagonists may provide addnl. dilatory benefit in cerebrovascular disorders associated with raised ET levels.

IT 162412-70-6, PD156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(endothelin-induced constriction in pial arteries from human brain and blockade and reversal)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

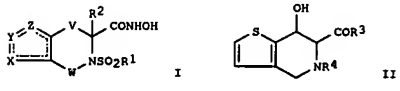
L4 ANSWER 64 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:113686 CAPLUS
DOCUMENT NUMBER: 130:182449
TITLE: Hydroxamic acid substituted fused heterocyclic metalloproteinase inhibitors
INVENTOR(S): Thomson, David S.; Koch, Kevin; Hwang, Chan Kou; Russo-Rodriguez, Sandra E.; Hummel, Conrad
PATENT ASSIGNEE(S): Amgen Inc., USA
SOURCE: PCT Int. Appl., 428 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906410	A1	19990211	WO 1998-US16147	19980804
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2297988	A1	19990211	CA 1998-2297988	19980804
AU 9887664	A	19990222	AU 1998-87664	19980804
EP 1003751	A1	20000531	EP 1998-939182	19980804
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003524572	T	20030819	JP 2000-505168	19980804

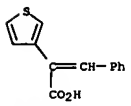
PRIORITY APPLN. INFO.:
US 1997-54753P P 19970804
US 1998-128512 A 19980803
WO 1998-US16147 W 19980804

OTHER SOURCE(S): MARPAT 130:182449
GI



AB Hydroxamic acid substituted fused heterocyclic compds. I [R1 = (un)substituted aliphatic cycloalkyl, heterocyclic; R2 = H, alkyl; V = (un)substituted CH2, CH2CH2; WN = CON, (un)substituted COCH2N, CH2N, CH2CH2N; X = O, S, Y = (un)substituted CH, Z = N, (un)substituted CH; Y = O, S, X, Z = (un)substituted CH; Z = O, S, X = N, (un)substituted CH, Y = (un)substituted CH] are effective for prophylaxis and treatment of inflammation, tissue degradation and related diseases. Thus, 2-thiophenecarboxaldehdye was treated with glycine and cyclized with CH2O to give the thienopyridine II [R3 = OH, R4 = H] which was

L4 ANSWER 64 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
4-methoxybenzenesulfonylated, O-acetylated, treated with NH2OH, and deacetylated to give II [R3 = NHOH, R4 = SO2C6H4OMe-4]. I are inhibitors of tumor necrosis factor convertase, human neutrophil collagenase, and human fibroblast stromelysin.
IT 50920-07-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thia- and oxaazabicycloalkanecarbohydroxamic acids as metalloproteinase inhibitors)
RN 50920-07-5 CAPLUS
CN 3-Thiopheneacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

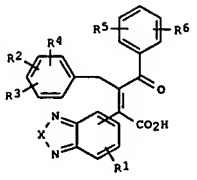
L4 ANSWER 65 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:81670 CAPLUS
DOCUMENT NUMBER: 130:139346
TITLE: Preparation of benzothiadiazolylbenzyloxobutenoates as endothelin receptor antagonists.
INVENTOR(S): Dorsch, Dieter; Osswald, Mathias; Mederski, Werner; Wilm, Claudia; Christadler, Maria; Schmitges, Claus J.
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19731571	A1	19990128	DE 1997-19731571	19970723
CA 2297315	A1	19990204	CA 1998-2297315	19980629
WO 9905132	A1	19990204	WO 1998-EP3957	19980629
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9888022	A	19990216	AU 1998-88022	19980629
AU 733338	B2	20010510		
EP 1000044	A1	20000517	EP 1998-939552	19980629
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
BR 9811537	A	20000829	BR 1998-11537	19980629
HU 200003335	A2	20010730	HU 2000-3335	19980629
JP 2001510836	T	20010807	JP 2000-504129	19980629
TW 461887	B	20011101	TW 1998-87111803	19980720
IN 1998CA01261	A	20050311	IN 1998-CA1261	19980720
ZA 9806551	A	19990920	ZA 1998-6551	19980722
NO 2000000324	A	20000121	NO 2000-324	20000121
US 6197800	B1	20010306	US 2000-463311	20000327

PRIORITY APPLN. INFO.: DE 1997-19731571 A 19970723
WO 1998-EP3957 W 19980629

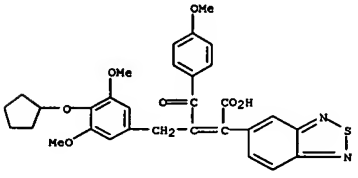
OTHER SOURCE(S): MARPAT 130:139346
GI

L4 ANSWER 65 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



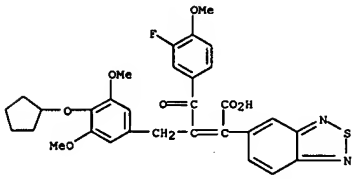
I

AB Title compds. [I; X = O, S; R1 = H, halo, A, OA; R2, R3, R5, R6 = H, halo, A, OA, R4; R4 = O(CH2)nCy; Cy = C3-8 cycloalkyl; A = (O-, S-, or CR5:CR5-interrupted) (fluorinated) alkyl; n = 0-2; and tautomeric ring closed forms], were prepared as drugs (no data). Thus, 4-cyclopentyloxy-3,5-dimethoxybenzaldehyde, and Me 2-(2,1,3-benzothiadiazol-5-yl)-4-(4-methoxyphenyl)-4-oxobutanoate (preparation given) were refluxed in EtOH containing NaOEt to give 3-(2,1,3-benzothiadiazol-5-yl)-4-(4-cyclopentyloxy-3,5-dimethoxybenzyl)-5-hydroxy-5-(4-methoxyphenyl)-5H-furan-2-one.
IT 219993-82-5P 219993-83-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzothiadiazolylbenzyloxobutenoates as endothelin receptor antagonists)
RN 219993-82-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



RN 219993-83-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(cyclopentyloxy)-3,5-dimethoxyphenyl]methyl]-2-(3-fluoro-4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 65 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



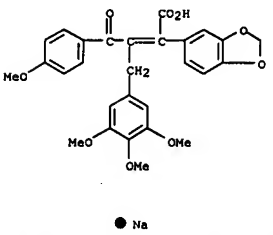
L4 ANSWER 66 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:30246 CAPLUS
DOCUMENT NUMBER: 130:246639
TITLE: Macrophage and myofibroblast involvement in ischemic acute renal failure is attenuated by endothelin receptor antagonists
AUTHOR(S): Forbes, Josephine M.; Leaker, Brian; Hewitson, Tim D.; Becker, Gavin J.; Jones, Colin L.
CORPORATE SOURCE: Victorian Paediatric Renal Service, Royal Children's Hospital, Parkville, Australia
SOURCE: Kidney International (1999), 55(1), 198-208
CODEN: KDYIA5; ISSN: 0085-2538
PUBLISHER: Blackwell Science, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Endothelin (ET) may be a mediator of injury following ischemia-induced acute renal failure (ARF). ET receptor (ETR) antagonists have been reported to increase survival rates and lower serum creatinines when administered postrenal ischemia-reperfusion injury in the rat. Renal cellular and extracellular matrix responses to this therapy have not been addressed. We investigated the use of ETR antagonists, PD 156707 (ETA) and SB 209670 (ETA and ETB) in the treatment of sublethal postischemic ARF. The right kidney of female Sprague-Dawley rats weighing approx. 200 g was removed. After five days, the left renal pedicle was occluded for 45 min. Twenty-four hours after renal ischemia, one of two ETR antagonists, PD 156707 (N = 7) or SB 209670 (N = 8), was administered. Exptl. animals were compared with an ischemic group receiving only saline (N = 9). Three nephrectomized groups that did not undergo ischemia but that received infusions of saline (N = 6), PD 156707 (N = 6), and SB 209670 (N = 6), resp., were also studied. Animals were sacrificed one week postischemia. Quantitation of monocytes and macrophages (Mo/Mϕ), α-smooth muscle actin-pos. myofibroblasts, and collagens type III and IV was performed by immunohistochem. staining. Cell kinetics were examined by staining for apoptosis with terminal deoxyuridine triphosphate (dUTP) nick end labeling and for proliferation with proliferating cell nuclear antigen. All ischemic groups of rats initially developed raised serum creatinine levels; however, no significant difference was observed between the groups (Kruskal-Wallis). Creatinines returned to preischemic values in all groups by the time of sacrifice. No significant difference in kidney wts. or body wts. was found between groups. Histol., infiltration of Mo/Mϕ was significantly reduced in groups treated with ETR antagonists (P < 0.001). The presence of myofibroblasts was also significantly reduced in the antagonist-treated groups (P < 0.001). This was also paralleled by reduced quantities of collagen IV in the treated rat groups (P < 0.001). The interstitial area was also significantly greater in the saline group (P < 0.001). The amount of collagen III did not significantly differ between rat groups. Apoptosis was reduced (P < 0.001) by treatment with ETR antagonists, whereas proliferation was enhanced (P < 0.005). All non-ischemic groups showed no variation in any parameter studied at this time point. Treatment of ischemic ARF in the rat with ETR antagonists PD 156707 and SB 209670 attenuated cellular infiltration and matrix accumulation. An advantage of one antagonist over

L4 ANSWER 66 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

the other could not be detd. in this study. The marked discrepancy between function and pathol. (former unchanged, latter markedly improved) may be due to the time frame of this expt., and longer outcome measures need to be assessed.

IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(macrophage and myofibroblast involvement in ischemic acute renal failure attenuated by endothelin receptor antagonists)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



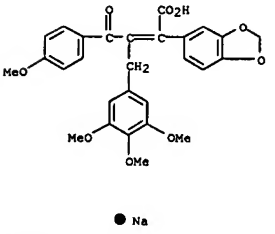
REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 67 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:21240 CAPLUS
DOCUMENT NUMBER: 130:204606
TITLE: The therapeutic potential of PD156707 and related butenolide endothelin antagonists
AUTHOR(S): Maguire, Janet J.; Davenport, Anthony P.
CORPORATE SOURCE: Clinical Pharmacology Unit, Centre for Clinical Investigation, Addenbrooke's Hospital, Cambridge, CB2 2QQ, UK
SOURCE: Expert Opinion on Investigational Drugs (1999), 8(1), 71-78
CODEN: EOIDER; ISSN: 1354-3784
PUBLISHER: Ashley Publications
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review, with 65 refs. Plasma concns. of the peptide endothelin (ET) are elevated in several cardiovascular diseases. Animal studies suggest that activation of ET receptors may contribute to the increase in vascular resistance and remodelling of cardiovascular tissues that are characteristic of these pathologies. Antagonists of these receptors may therefore have important clin. potential. PD156707 (Parke-Davis) is one of a series of novel, orally-active butenolide endothelin antagonists and is highly selective for the ETA receptor. In man, this subtype mediates the profound vasoconstrictor effects of the ET peptides, and blockade of the ETA receptor may therefore produce beneficial vasodilatation. The advantage of selective ETA receptor antagonism is that it leaves unaffected vascular ETB receptors, which mediate vasorelaxation, and non-vascular ETB receptors, particularly in the lung and kidneys, which act to clear ET from the plasma. PD156707 exhibits subnanomolar affinity and greater than 1000-fold selectivity for human ETA receptors and potently inhibits ET-1-mediated vasoconstriction in human isolated blood vessels. In rats, PD156707 has good oral bioavailability (41%) and a relatively short terminal t1/2 of approx. 1 h. Structural analogs of PD156707 that have comparable selectivity and potency for the ETA receptor are reported to have even better oral bioavailability and longer plasma t1/2 values. Preclin. studies with PD156707 indicate efficacy in animal models of congestive heart failure (CHF), pulmonary hypertension (PH) and cerebral ischemia. The authors await data from clin. trials to confirm the therapeutic potential of the ETA-selective butenolide antagonists in man.

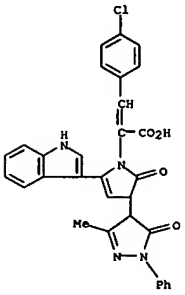
IT 162412-70-6, PD156707
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(PD156707 and related butenolide endothelin antagonists therapeutic potential in cardiovascular diseases in humans)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 67 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



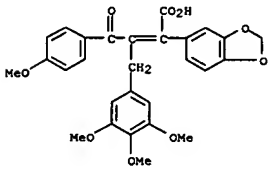
REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 68 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:725980 CAPLUS
DOCUMENT NUMBER: 130:153625
TITLE: Reactivity of pyrrolinone derivatives towards some electrophiles and nucleophiles
AUTHOR(S): Kassab, Rafika R.
CORPORATE SOURCE: Chemistry Department Faculty of Science, Al-Azhar (for girls) University, Nasr City, Egypt
SOURCE: Al-Azhar Bulletin of Science (1997), 8(2), 299-307
CODEN: ABSCE7; ISSN: 1110-2535
PUBLISHER: Al-Azhar University, Faculty of Science
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A [(1H-indol-3-yl)oxopyrrolyl]pyrazolone derivative was prepared and reaction products with various substrates were described.
IT 220259-53-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 220259-53-0 CAPLUS
CN 1H-Pyrrole-1-acetic acid, α-[(4-chlorophenyl)methylene]-3-(4,5-dihydro-3-methyl-5-oxo-1-phenyl-1H-pyrazol-4-yl)-2,3-dihydro-5-(1H-indol-3-yl)-2-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 69 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:698832 CAPLUS
DOCUMENT NUMBER: 130:104586
TITLE: Discovery and development of an endothelin A receptor-selective antagonist PD 156707
AUTHOR(S): Doherty, Annette M.; Uprichard, Andrew C. G.
CORPORATE SOURCE: Department of Chemistry, Parke-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Pharmaceutical Biotechnology (1998), 11(Integration of Pharmaceutical Discovery and Development), 81-112
CODEN: PHBIEB; ISSN: 1078-0467
PUBLISHER: Plenum Publishing Corp.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with many refs. on the development of nonpeptide endothelin antagonists and the discovery of the clin. candidate PD 156707. PD 156707 is a highly potent selective antagonist of the endothelin A (ETA) receptor that has demonstrated efficacy in a number of different disease models.
IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(discovery and development of endothelin A receptor-selective antagonist PD 156707)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



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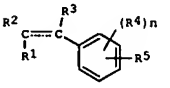
REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 69 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
FORMAT

L4 ANSWER 70 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:693417 CAPLUS
DOCUMENT NUMBER: 129:343326
TITLE: Preparation of benzenes as protein kinase C inhibitors
INVENTOR(S): Mori, Toyoki; Tominaga, Michiaki; Tabusa, Fujio; Ei, Kazuyoshi; Nakaya, Kenji; Takemura, Isao; Shinohara, Tomokazu; Tanada, Yoshihisa; Yamauchi, Takahito; Kitano, Kazuyoshi
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 359 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10287634	A	19981027	JP 1997-110527	19970411
PRIORITY APPLN. INFO.:			JP 1997-110527	19970411

OTHER SOURCE(S): MARPAT 129:343326
GI



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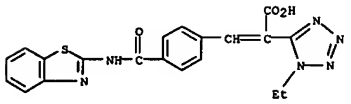
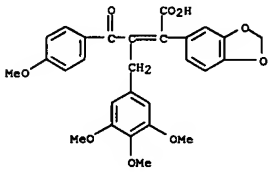
AB Benzenes I [R1 = 5- to 6-membered (un)substituted unsatd. heterocyclyl having 1-4 N, O, or S; cyano, carboxylalkyl, alkoxycarbonyl, H, Bz, (un)substituted amido, etc.; R2 = (un)substituted Bz, (un)substituted 1,2,3,4-tetrahydroquinolinylcarbonyl, pyridylcarbonyl, (un)substituted phenoxycarbonyl, etc.; R3 = H, lower alkyl, PhS, (un)substituted lower alkylthio, cycloalkylthio, cyano, etc.; R4 = H, (un)substituted lower alkyl, lower alkoxy, (un)substituted aminoalkylene, (un)substituted aminoalkylenyloxy; R5 = substituted alkenyl, phenylthioureidocarbonyl, pyrimidylaminocarbonylalkoxy, etc.; n = 1-3; the dot line may be double bond] or their salts are prepared I are useful for prevention and treatment of chronic rheumatoid arthritis, systemic lupus erythematosus, atopic dermatitis, heart failure, allergy, multiple sclerosis, tumor, Alzheimer-type dementia, etc. Condensation of 250 mg 2-(benzoylmethyl)pyridine with 300 mg 4-[(2-benzothiazolyl)aminocarbonyl]benzaldehyde in C6H6 for 10 h gave 0.3 g 2-[4-[2-benzoyl-2-(2-pyridyl)vinyl]benzoylamino]benzothiazole.
IT 215506-69-7P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzenes as protein kinase C inhibitors for treatment of

L4 ANSWER 70 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
diseases)
RN 215506-69-7 CAPLUS
CN 1H-Tetrazole-5-acetic acid, α-[[4-[(2-benzothiazolylamino)carbonyl]phenyl]methylene]-1-ethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 71 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:689025 CAPLUS
DOCUMENT NUMBER: 130:89900
TITLE: PD-156707: a selective endothelin-A receptor antagonist
AUTHOR(S): Uprichard, Andrew C. G.; Metz, Alan L.; Hallak, Hussein; Haleen, Stephen J.
CORPORATE SOURCE: Parke-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Cardiovascular Drug Reviews (1998), 16(2), 89-104
CODEN: CDREEA; ISSN: 0897-5957
PUBLISHER: Neva Press
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 59 refs. PD-156707 is a highly potent, specific antagonist of the endothelin-A (ETA) receptor discovered as the result of directed structure-activity studies and lead optimization of a chemical library screen
hit. Despite a short terminal elimination half-life, the drug good oral bioavailability and is well suited to chronic oral dosing. The drug has been tested in a number of whole-animal disease models with efficacy demonstrated in heart failure, stroke and pulmonary hypertension.
IT 162412-70-6, PD-156707
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC
(Process); USES (Uses)
(pharmacol. of PD-156707 as selective endothelin-A receptor antagonist)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



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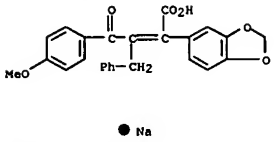
REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 71 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 72 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:647140 CAPLUS
DOCUMENT NUMBER: 130:33410
TITLE: Evaluation of the effect of endothelin-1 and characterization of the selective endothelin A receptor antagonist PD155080 in the prostate
AUTHOR(S): Imajo, Chieko; Walden, Paul D.; Shapiro, Ellen; Doherty, Annette M.; Lepor, Herbert
CORPORATE SOURCE: Department of Urology, Biochemistry and Pharmacology, New York University Medical Center, NY, USA
SOURCE: Journal of Urology (Baltimore) (1997), 158(1), 253-257
CODEN: JOURAA; ISSN: 0022-5347
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The purpose of this study was to evaluate the contractile effect of endothelin-1 (ET-1) on prostatic urethral pressure and to characterize the
effect of the selective ETA receptor antagonist PD155080 on ET-1 mediated prostatic urethral pressure. The effect of i.v. ET-1 administration on canine urethral pressure was determined in the presence and absence of PD155080. The affinity of PD155080 for endothelin mediated contraction was determined using antagonist dissociation studies. Saturation and competition
binding studies were performed using [125I] ET-1 in both human and canine prostate. ET-1 bolus injection elicited shallow and prolonged increases in the prostatic urethral pressure. Pretreatment with PD155080 totally abolished the urethral contractile response to ET-1. Specific [125I] ET-1
binding was saturable and of high affinity. Two ET receptor subtypes (ETA
receptor, ETB receptor) have been identified in human prostate. The ratio
of ETA to ETB receptors was approx. 1.5:1 in both human and canine prostates. Isometric tension studies revealed that PD155080 shifted the ET-1 dose-response curves to the right and exhibited no effect on the ETB receptor selective agonist sarafotoxin dose-response curves. ET-1 mediates prostate smooth muscle tone and may play a role in the pathophysiol. and treatment of benign prostatic hyperplasia (BPH).
IT 162412-71-7, PD155080
RL: BAC (Biological activity or effector, except adverse); BPR (Biological
process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(endothelin-1 contractile effect and characterization of selective endothelin A receptor antagonist PD155080 in prostates of dogs and humans)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 72 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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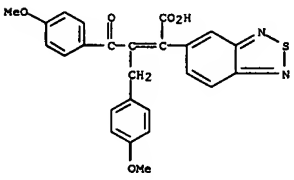
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

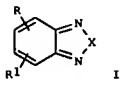
L4 ANSWER 73 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
methoxyphenyl)-4-oxobutanoate (prepn. given) were refluxed in MeOH contg. NaOMe followed by addn. of HOAc and further reflux to give 3-(2,1,3-benzothiadiazol-5-yl)-4-benzyl-5-hydroxy-5-(4-methoxyphenyl)-5H-furan-2-one.
IT 195505-54-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzothiadiazolylfuranones and related compds. as endothelin
receptor antagonists)
RN 195505-54-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-methoxyphenyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



L4 ANSWER 73 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:640521 CAPLUS
DOCUMENT NUMBER: 129:260463
TITLE: Preparation of benzothiadiazolylfuranones and related compounds as endothelin receptor antagonists.
INVENTOR(S): Dorsch, Dieter; Mederski, Werner; Schmitges, Claus-Jochen; Oswald, Mathias; Wilm, Claudia; Christadler, Maria
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany
SOURCE: Ger. Offen., 32 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19712141	A1	19980924	DE 1997-19712141	19970322
WO 9842702	A1	19981001	WO 1998-EP1204	19980304
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9868263	A	19981020	AU 1998-68263	19980304
ZA 9802370	A	19980923	ZA 1998-2370	19980319
IN 1998CA00469	A	20050805	IN 1998-CA469	19980320
PRIORITY APPLN. INFO.:			DE 1997-19712141 A	19970322
			WO 1998-EP1204 W	19980304

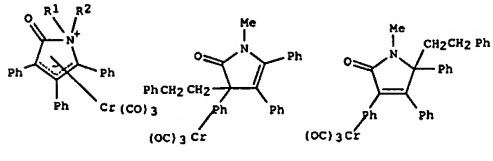
OTHER SOURCE(S): MARPAT 129:260463
GI



I

AB Title compds. [I; R = specified (substituted) furanone group; R1 = H, halo, OH, OA, SA, SOA, SO2A, NO2, amino, acylamino, CHO, CO2A, CH2CO2H, etc.; A = (O- or S-interrupted) alkyl, alkenyl; X = O, S], were prepared for
treatment of hypertension, heart failure, kidney failure, coronary heart disease, renal, cerebral, and myocardial ischemia, subarachnoid hemorrhage, inflammation, asthma, endotoxic shock, and brain infarct (no data). Thus, PhCHO and Et 2-(2,1,3-benzothiadiazol-5-yl)-4-(4-

L4 ANSWER 74 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:626713 CAPLUS
DOCUMENT NUMBER: 130:3927
TITLE: Reaction of aminocarbene complexes of chromium with alkynes. 9. From nitrogen ylide complexes toward alkaloid frameworks
AUTHOR(S): Rudler, Henri; Parlier, Andree; Rudler, Michele; Vaissermann, Jacqueline
CORPORATE SOURCE: UMR 7611, Laboratoire de Synthese Organique et Organometallique, Universite Pierre et Marie Curie, Paris, 75252, Fr.
SOURCE: Journal of Organometallic Chemistry (1998), 567(1-2), 101-118
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:3927
GI



I II III

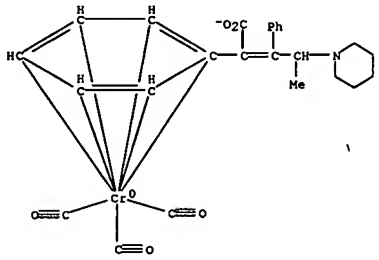
AB Aminocarbene complexes of chromium having the general structure (CO)5Cr:C(R)NR1R2 react with diphenylacetylene to give pyrrolinones as the
result of the insertions of the alkyne, of CO and the migration of an alkyl group from nitrogen to a carbon atom in α or γ with respect to the nitrogen atom. The mechanism of this new reaction has been
thoroughly investigated: a nitrogen ylide originating from the interaction
of the nitrogen atom of the starting aminocarbene complex with the central
carbon of the ketene formed by insertion of the alkyne and of CO into the aminocarbene complex, is a crucial intermediate in these reactions. This ylide complex, the structure of which could be established as I, leads to the observed pyrrolinones upon thermolysis. Mechanisms involving radicals
have been discarded on the grounds of the reaction of cyclopropylcarbinyl-
substituted aminocarbene complexes: no rearrangement of the cyclopropylcarbinyl group is observed upon its migration, as shown by the x-ray structure of the pyrrolinone. Mechanisms involving ion pairs or the
participation of the metal have also been eliminated. For that purpose,

L4 ANSWER 74 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
the x-ray structures of two complexes, II and III, in which the metal is not bound to the Ph ring of the migrating groups, have been established. Finally, concerted (1,5) sigmatropic migrations of the alkyl groups from nitrogen to the carbons of the five-membered heterocycle in I account best for the obsd. results. The role of the metal could also be detd. by the examn. of the reactivity of the metal-free N-ylides. No rearrangement similar to that obsd. for complexes I is obsd.; only products arising from the cleavage of the bond between nitrogen and the central carbon of the ketene were obtained. As an application of this original reaction of carbene complexes, the synthesis of derivs. of the lycorine alkaloid will be described: the keypoint is the use of intramol. insertions of alkynes into suitably substituted aminocarbene complexes of chromium.

IT 131374-61-3P 131374-63-5P 215777-73-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 131374-61-3 CAPLUS
CN Chromate(1-), tricarbonyl[(1,2,3,4,5,6-η)-α-[(1E)-1-phenyl-2-(1-piperidinyl)propylidene]benzeneacetato]-, hydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

● H+

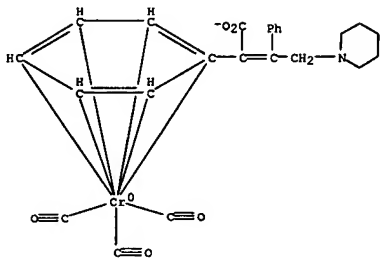
RN 131374-63-5 CAPLUS
CN Chromate(1-), tricarbonyl[(1,2,3,4,5,6-η)-α-[(1E)-1-phenyl-2-(1-piperidinyl)ethylidene]benzeneacetato]-, hydrogen (9CI) (CA INDEX NAME)

L4 ANSWER 74 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PAGE 2-A

● H+

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 74 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
PAGE 1-A

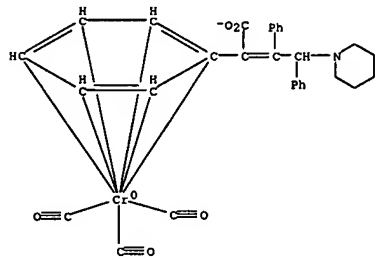


PAGE 2-A

● H+

RN 215777-73-4 CAPLUS
CN Chromate(1-), tricarbonyl[(1,2,3,4,5,6-η)-α-[1,2-diphenyl-2-(1-piperidinyl)ethylidene]benzeneacetato]-, hydrogen (9CI) (CA INDEX NAME)

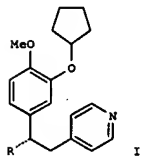
PAGE 1-A



L4 ANSWER 75 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:604712 CAPLUS
DOCUMENT NUMBER: 129:245046
TITLE: Method of preparing phosphodiesterase IV inhibitors
INVENTOR(S): Choi, Woo-Baeg; Churchill, Hywyn R. O.; Lynch, Joseph E.; Reider, Paul J.; Volante, Ralph P.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 18 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5808082	A	19980915	US 1997-837733	19970422
PRIORITY APPLN. INFO.:			US 1997-837733	19970422

OTHER SOURCE(S): CASREACT 129:245046; MARPAT 129:245046
GI

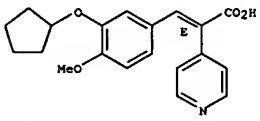


AB A process for the preparation of phosphodiesterase IV inhibitors [I; R1 = Ph, (un)substituted aryl, etc.] is described. The process consists of eight chemical steps involving five isolations to prepare the title compound from readily available isovanillin in 35% overall yield. The process is highlighted by: (a) a highly diastereoselective Michael addition of phenyllithium using (1R,2S) cis-aminoindanol as a chiral auxiliary, (b) highly crystalline intermediates providing for efficient purifications, (c) crystallization of the final compound as its CSA salt for excellent enantiomeric purity.

IT 199331-21-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyridine derivs. as phosphodiesterase IV inhibitors)

RN 199331-21-0 CAPLUS
CN 4-Pyridineacetic acid, α-[[3-(cyclopentyloxy)-4-methoxyphenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

L4 ANSWER 75 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



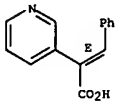
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 76 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:586326 CAPLUS
DOCUMENT NUMBER: 129:230648
TITLE: Preparation of pyridylpropionylguanidines as Na+/H+ exchange inhibitors
INVENTOR(S): Okazaki, Toshio; Kikuchi, Kazumi; Kako, Hideki; Takanashi, Masahiro
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan; Merck Patent G.m.b.H.
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10237077	A	19980908	JP 1997-42420	19970226
PRIORITY APPLN. INFO.:			JP 1997-42420	19970226

OTHER SOURCE(S): MARPAT 129:230648
GI For diagram(s), see printed CA Issue.
AB Title compds. I [ring A = (substituted) 5- to 6-membered heteroaryl; ring B = (substituted) aryl; R1-R3 = H, (F-substituted) lower alkyl] and their salts, useful as antihypertensives, antiarrhythmic agents, antianginal agents, etc., are prepared HN:C(NH2)2.HCl (1.00 g) was reacted with MeONa in MeOH at room temperature for 5 min and amidated with 0.40 g 3-phenyl-2-(3-pyridyl)propanoic acid (preparation given) in the presence of 1,1'-carbonyl-bis(1-H-imidazole) in DMF at room temperature for 15 min to give 0.29 g N-[3-phenyl-2-(3-pyridyl)propionyl]guanidine.
IT 141694-17-9P 188815-49-8P 188815-55-6P 188815-68-1P 212792-92-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyridylpropionylguanidines as Na+/H+ exchange inhibitors)
RN 141694-17-9 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

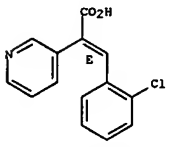
Double bond geometry as shown.



RN 188815-49-8 CAPLUS

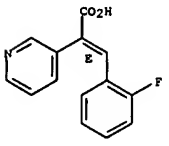
L4 ANSWER 76 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 3-Pyridineacetic acid, α-[(2-chlorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



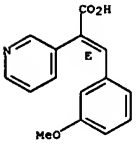
RN 188815-55-6 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-fluorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-68-1 CAPLUS
CN 3-Pyridineacetic acid, α-[(3-methoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

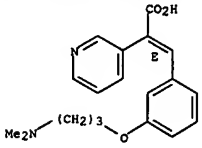
Double bond geometry as shown.



RN 212792-92-2 CAPLUS
CN 3-Pyridineacetic acid, α-[[3-[3-(dimethylamino)propoxy]phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 76 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

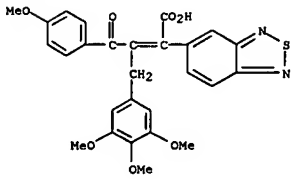


L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:482712 CAPLUS
DOCUMENT NUMBER: 129:211231
TITLE: Endothelin antagonists: discovery of EMD 122946, a highly potent and orally active ETA selective antagonist
AUTHOR(S): Mederski, Werner W. K. R.; Dorsch, Dieter; Osswald, Mathias; Anzali, Soheila; Christadler, Maria; Schmitges, Claus-Jochen; Schelling, Pierre; Wilm, Claudia; Fluck, Markus
CORPORATE SOURCE: Merck KGaA, Preclinical Pharmaceutical Research, Darmstadt, 64271, Germany
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998), 8(13), 1771-1776
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The discovery, in vitro and in vivo studies of the highly potent ETA antagonist benzothiadiazole EMD 122946 are presented. Structure-activity relations of the benzothiadiazoles as selective ETA antagonists are presented. EMD 122946 displayed high binding affinity and functional antagonism [IC50 = 3.2+10-11 M, pA2 = 9.5 (ETA)] and inhibited the ET-1 induced pressor response in pithed rats with an ED50 of 0.3 mg/kg. In conscious spontaneously hypertensive rats and in DOCA-salt hypertensive rats the compound lowered mean blood pressure with an ED50 of 0.06 mg/kg. EMD 122946 exhibited high bioavailability in rats and monkeys.

IT 195505-82-9P, EMD 122801
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(discovery of benzothiadiazole EMD 122946 as highly potent and orally active ETA endothelin selective antagonist with antihypertensive activity in relation to structure-activity relations)

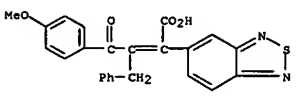
RN 195505-82-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

IT 195505-81-8P 195505-86-3P 195505-87-4P
195505-94-3P, EMD 122946 212390-67-5P
212390-68-6P 212390-69-7P 212390-70-0P
212390-71-1P 212390-72-2P 212390-74-4P
212390-76-6P 212390-78-8P 212390-79-9P
212390-80-2P 212390-81-3P 212390-82-4P
212390-83-5P 212390-84-6P 212390-85-7P
212390-86-8P 212390-87-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(discovery of benzothiadiazole EMD 122946 as highly potent and orally active ETA endothelin selective antagonist with antihypertensive activity in relation to structure-activity relations)

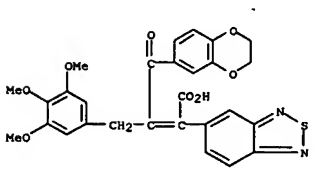
RN 195505-81-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

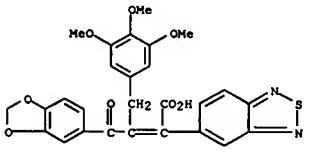
RN 195505-86-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-,

sodium salt (9CI) (CA INDEX NAME)



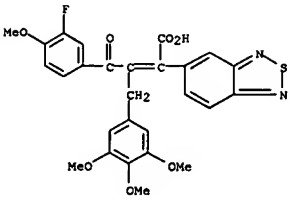
● Na

RN 195505-87-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(1,3-benzodioxol-5-yl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



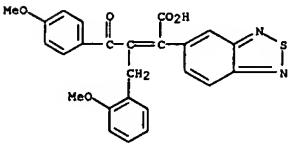
● Na

RN 195505-94-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

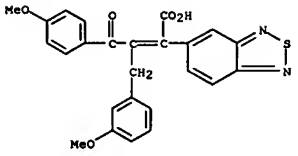
RN 212390-67-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(2-methoxyphenyl)methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

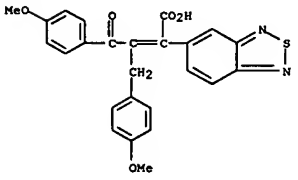
RN 212390-68-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(3-methoxyphenyl)methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

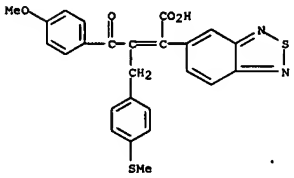
RN 212390-69-7 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-methoxyphenyl)methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

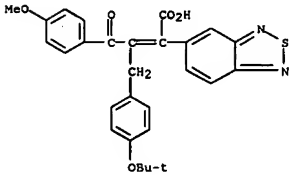
RN 212390-70-0 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[[4-(methylthio)phenyl]methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

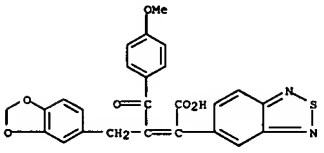
RN 212390-71-1 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(1,1-dimethylethoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

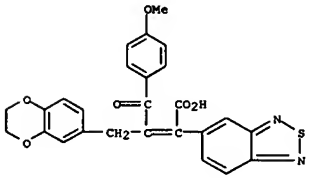
RN 212390-72-2 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-(1,3-benzodioxol-5-ylmethyl)-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

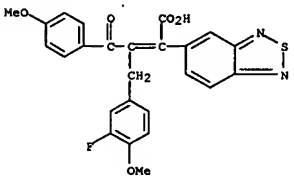
RN 212390-74-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

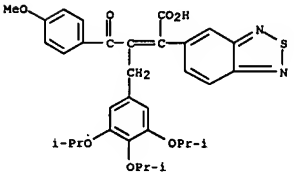
RN 212390-76-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[(3-fluoro-4-methoxyphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

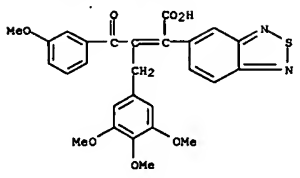
RN 212390-78-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[[3,4,5-tris(1-methylethoxy)phenyl]methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

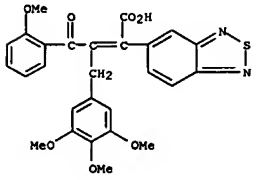
RN 212390-79-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

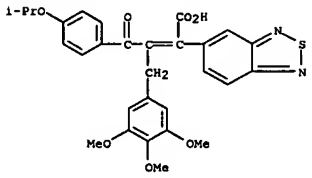
RN 212390-80-2 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

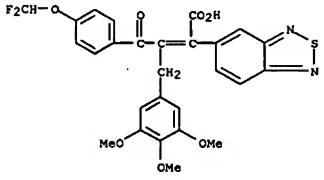
RN 212390-81-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-[4-(1-methylethoxy)phenyl]-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

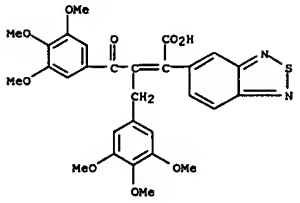
RN 212390-82-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-[4-(difluoromethoxy)phenyl]-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

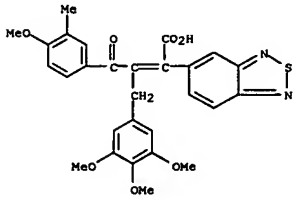
RN 212390-83-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-oxo-2-(3,4,5-trimethoxyphenyl)-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

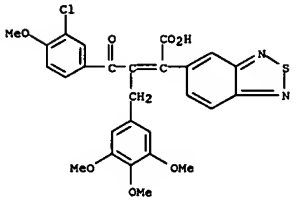
RN 212390-84-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

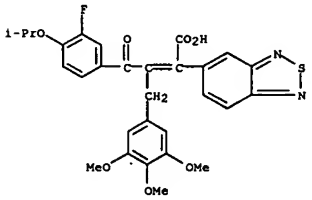
RN 212390-85-7 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-chloro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

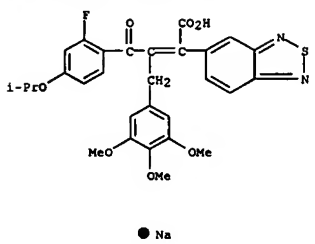
RN 212390-86-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-[3-fluoro-4-(1-methylethoxy)phenyl]-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

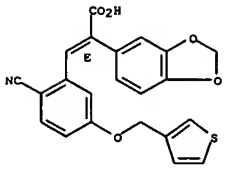
RN 212390-87-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-[2-fluoro-4-(1-methylethoxy)phenyl]-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 77 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 78 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 78 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:446681 CAPLUS
DOCUMENT NUMBER: 129:108875
TITLE: Selective Endothelin A Receptor Antagonists. 4. Discovery and Structure-Activity Relationships of Stilbene Acid and Alcohol Derivatives
AUTHOR(S): Astles, Peter C.; Brown, Thomas J.; Halley, Frank; Handscombe, Caroline M.; Harris, Neil V.; McCarthy, Clive; McLay, Iain M.; Lockey, Peter; Majid, Tahir; Porter, Barry; Roach, Alan G.; Smith, Christopher; Walsh, Roger
CORPORATE SOURCE: Dagenham Research Centre, Rhone-Poulenc Rorer, Dagenham, Essex, RM10 7XS, UK
SOURCE: Journal of Medicinal Chemistry (1998), 41(15), 2745-2753
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This publication describes the synthesis and optimization of a novel series of stilbene endothelin antagonists. Anal. of the SAR established for previous papers in this series prompted the design and synthesis of (Z)-4-phenyl-5-(3-benzyloxyphenyl)pent-4-enoic acid (3), which was found to be a moderately active inhibitor of the binding of [125I]ET-1 to ETA receptors with an IC50 of 6 μM. More interestingly, the intermediate compound (E)-2-phenyl-3-(3-benzyloxyphenyl)propenoic acid (5) was equiactive with 3. Optimization of 5 resulted in the preparation of (E)-2-phenyl-3-(2-cyano-5-(thien-3-ylmethoxy))phenylpropenoic acid (RPR111723), which had an IC50 in the binding assay of 80 nM on the ETA receptor and a pKB of 6.5 in the functional assay, measured on rat aortic strips. Reduction of the acid group of 5 gave the first nonacidic ETA antagonist in our series, (E)-2-phenyl-3-(3-benzyloxyphenoxy)prop-2-enol (6) with an IC50 of 20 μM. Optimization of 6 resulted in the preparation of 2-(2-methylphenyl)-3-(2-cyano-5-(thien-3-ylmethyl)phenyl)prop-2-enol with an IC50 of 300 nM on the ETA receptor.

IT 210109-80-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of stilbene acid and alc. derivs. as endothelin A receptor antagonists)

RN 210109-80-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[[2-cyano-5-(3-thienylmethoxy)phenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 79 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:424239 CAPLUS
DOCUMENT NUMBER: 129:81735
TITLE: Preparation of benzothiadiazolyloxobutenoates and analogs as endothelin receptor antagonists
INVENTOR(S): Dorsch, Dieter; Osswald, Mathias; Mederski, Werner; Wilm, Claudia; Schmitges, Claus Jochen; Christadler, Maria; Anzali, Soheila
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany; Dorsch, Dieter; Osswald, Mathias; Mederski, Werner; Wilm, Claudia; Schmitges, Claus Jochen; Christadler, Maria; Anzali, Soheila
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9827077	A1	19980625	WO 1997-EP7045	19971215
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19653037	A1	19980625	DE 1996-19653037	19961219
AU 9856635	A	19980715	AU 1998-56635	19971215
IN 1997CA02400	A	20050311	IN 1997-CA2400	19971218
PRIORITY APPLN. INFO.:			DE 1996-19653037 A	19961219
			WO 1997-EP7045 W	19971215

OTHER SOURCE(S): MARPAT 129:81735
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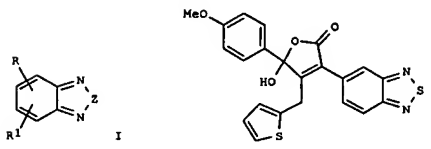
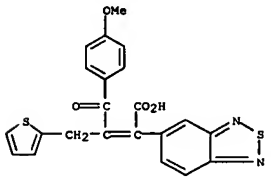
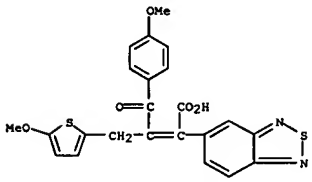


AB Title compds. [tautomeric I; R = C(CO2H):C(COR3)(CH2)nR2, COC[(CH2)nR2]:CR4CO2H, (CH2)nC(COR3):CR4CO2H; R1 = H, halo, alkyl, alkoxy, etc.; R2-R4 = (un)substituted Ph, etc.; R2 may addnl. = (cyclo)alkyl,

L4 ANSWER 79 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
etc.) were prepd. as endothelin receptor antagonists (no data). Thus, 3,4-(H2N)2C6H3CH2CO2Et was cyclocondensed with PhN:SO and the product alkylated by 4-(MeO)C6H4COCH2Br to give, in 2 addnl. steps, title compd. II.
IT 209345-15-3P 209345-16-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzothiadiazolyloxobutenoates and analogs as endothelin
receptor antagonists)
RN 209345-15-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(2-thienylmethyl)ethylidene]- (9CI) (CA INDEX NAME)



RN 209345-16-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(5-methoxy-2-thienyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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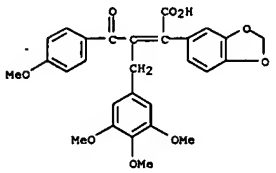
L4 ANSWER 80 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 80 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:312816 CAPLUS
DOCUMENT NUMBER: 129:49425
TITLE: PD156707: a potent antagonist of endothelin-1 in human
diseased coronary arteries and vein grafts
AUTHOR(S): Maguire, Janet J.; Davenport, Anthony P.
CORPORATE SOURCE: Clinical Pharmacology Unit, Addenbrooke's Hospital, University of Cambridge, Cambridge, CB2 2QQ, UK
SOURCE: Journal of Cardiovascular Pharmacology (1998), 31(Suppl. 1, Endothelin V), S239-S240
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott-Raven Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have determined the ability of the endothelin A (ETA)-selective antagonist
PD156707 to block constrictor ET-1 responses in blood vessels from the diseased human heart. ET-1 potently contracted nonatherosclerotic coronary arteries from patients with cardiomyopathy (pD2 = 7.96 ± 0.15; n = 6), atherosclerotic coronary arteries from patients with ischemic heart disease (pD2 = 8.26 ± 0.20; n = 4), and saphenous vein grafts that had developed "atherosclerotic" disease after coronary artery bypass (pD2 = 8.41 ± 0.09; n = 6). PD156707 (100 nM) antagonized the vasoconstrictor response to ET-1 in each of the three prepns., with estimated
pA2 values of 7.91 ± 0.20, 8.05 ± 0.14, and 8.07 ± 0.02, resp. These data suggest that the upregulation of ETB receptors that has been reported in human atherosclerotic coronary arteries does not contribute significantly to the ET-1-mediated constrictor response in these vessels in vitro.
IT 162412-70-6, PD156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(PD156707: a potent antagonist of endothelin-1 in human diseased coronary arteries and vein grafts)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX
NAME)

L4 ANSWER 81 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:300863 CAPLUS
DOCUMENT NUMBER: 129:4869
TITLE: Preparation of endothelin receptor-binding ultrasound contrast agents
INVENTOR(S): Klaveness, Jo; Naevestad, Anne; Cuthbertson, Alan; Solbakken, Magne
PATENT ASSIGNEE(S): Nycomed Imaging AS, Norway; Cockbain, Julian
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 10
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9818497	A2	19980507	WO 1997-GB2957	19971028
WO 9818497	A3	19980716		
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9747869	A	19980522	AU 1997-47869	19971028
EP 946202	A2	19991006	EP 1997-910517	19971028
EP 946202	B1	20030910		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AT 249247	T	20030915	AT 1997-910517	19971028
ES 2206689	T3	20040516	ES 1997-910517	19971028
US 2002102217	A1	20020801	US 2001-925715	20010810
US 6680047	B2	20040120		
US 2005002865	A1	20050106	US 2003-734730	20031215

PRIORITY APPLN. INFO.:

GB 1996-22364	A	19961028
GB 1996-22365	A	19961028
GB 1996-22366	A	19961028
GB 1996-22367	A	19961028
GB 1996-22368	A	19961028
GB 1996-22369	A	19961028
GB 1997-699	A	19970115
GB 1997-2195	A	19970204
GB 1997-9088	A	19970502
US 1997-48054P	P	19970530
GB 1997-8265	A	19970424
GB 1997-11837	A	19970606

L4 ANSWER 81 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

GB 1997-11839	A	19970606
US 1997-49264P	P	19970606
US 1997-49263P	P	19970607
US 1997-49266P	P	19970607
US 1997-959206	A	19971028
WO 1997-GB2957	W	19971028
US 2001-925715	A1	20010810

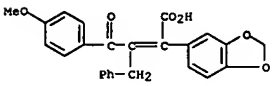
OTHER SOURCE(S): MARPAT 129:4869

AB Compns. of matter V-L-R (V is a non-peptidic organic group having binding affinity for an endothelin receptor site; L is a linker moiety or a bond; R is a moiety detectable in in vivo imaging of a human or animal body) are described. Thus, syntheses of Gd(III) and Tc chelates of a DPTA conjugate of a lysine conjugate of 27-O-3-[2-(3-carboxyacryloylamino)-5-hydroxyphenyl]acryloyloxymyricerone are described.

IT 207522-05-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of endothelin receptor-binding ultrasound contrast agents)

RN 207522-05-2 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)



L4 ANSWER 82 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:239195 CAPLUS
DOCUMENT NUMBER: 128:294774
TITLE: Improved process for synthesis of β-ketonitriles
INVENTOR(S): Davis, Edward Mark; Ellis, James E.
PATENT ASSIGNEE(S): Warner-Lambert Company, USA; Davis, Edward Mark; Ellis, James E.
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9815524	A1	19980416	WO 1997-US18159	19971007
W: AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, GH, HU, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9748116	A	19980505	AU 1997-48116	19971007
ZA 9709066	A	19980511	ZA 1997-9066	19971009
PRIORITY APPLN. INFO.:			US 1996-28439P	P 19961010
			WO 1997-US18159	W 19971007

OTHER SOURCE(S): CASREACT 128:294774; MARPAT 128:294774

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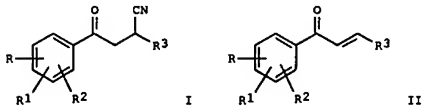


AB The title compds. I (R, R1, R2 = H, alkyl, alkoxy, amino, alkylamino, dialkylamino, aryl, halo, CO2 alkyl, CN, R3 = aryl, benzo[1,3]dioxol-5-yl) for use in preparation of endothelin-A (ETA) receptor antagonists are prepared by reacting α-β-enones II with acetone cyanohydrin (III) in the presence of tetraalkylammonium hydroxides. Preparation of hydroxybutenolides using β-ketonitriles is also provided. Thus, reacting 3-(benzo[1,3]dioxol-5-yl)-1-(4-methoxyphenyl)-prop-2-en-1-one with III gave 3-(benzo[1,3]dioxol-5-yl)-1-(4-methoxyphenyl)-4-oxobutyronitrile.

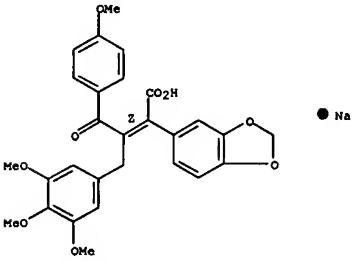
IT 206054-82-2P

L4 ANSWER 82 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(β-ketonitriles for prepn. of hydroxybutenolides for endothelin-A receptor antagonists)

RN 206054-82-2 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 83 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

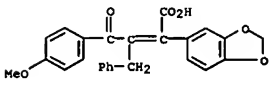
ACCESSION NUMBER: 1998:206316 CAPLUS
DOCUMENT NUMBER: 128:317090
TITLE: Stimulation of L-type Ca2+ current by the endothelin receptor A-selective antagonist, BQ-123, in ventricular cardiomyocytes isolated from rabbit myocardium
AUTHOR(S): Kelso, Elizabeth J.; Spiers, J. Paul; Mcdermott, Barbara J.; Scholfield, C. Norman; Silke, Bernard
CORPORATE SOURCE: Dep. Of Therapeutics And Pharmacology, The Queen's University Of Belfast, Belfast, BT9 7BL, UK
SOURCE: Biochemical Pharmacology (1998), 55(6), 897-902
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB BQ-123 is extensively used as an antagonist at endothelin (ET) receptors, having selectivity at the ETA receptor subtype. In this study, the effects of BQ-123 per se on action potentials, L-type calcium currents, and potassium currents, were examined in ventricular cardiomyocytes isolated from adult, male, New Zealand White rabbits, using the patch-clamp technique. BQ-123 (1 μM) increased ($P < 0.02$) the duration of the action potential to 267 ± 36 ms from a control duration of 228 ± 30 ms. BQ-123 did not have any effect on the inward rectifier or transient outward potassium currents, but increased ($P < 0.02$) the L-type Ca2+ current to -2.76 ± 0.3 nA from a control value of -2.45 ± 0.28 nA. The increases in both duration of the action potential and L-type Ca2+ current were reversed upon washout (233 ± 28 ms and -2.32 ± 0.31 nA, resp.) and were not different from the control values in the absence of BQ-123. In contrast, the endothelin receptor antagonists, BQ-788, PD155080 and PD145065 (1-10 μM) did not affect the L-type Ca2+ current. These results indicate that, unlike PD155080, BQ-788 and PD145065, the conventional ETA receptor-selective antagonist, BQ-123, exerts a unique pos. effect on the L-type Ca2+ current in ventricular cardiomyocytes isolated from rabbit myocardium. The mechanism of action of BQ-123, therefore, is not confined to ET receptor antagonism.

IT 162412-71-7, PD155080
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(comparison with; stimulation of L-type Ca2+ current by endothelin receptor A-selective antagonist, BQ-123, in ventricular cardiomyocytes isolated from rabbit myocardium)

RN 162412-71-7 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



L4 ANSWER 83 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

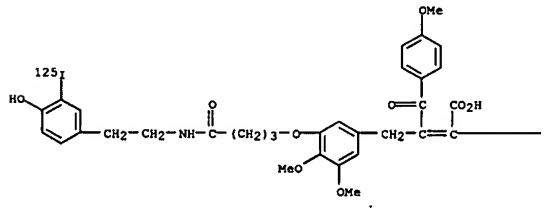
L4 ANSWER 84 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:82205 CAPLUS
DOCUMENT NUMBER: 128:212966
TITLE: Characterization of [125I]-PD-164333, an ETA selective
non-peptide radiolabeled antagonist, in normal and diseased human tissues
AUTHOR(S): Davenport, Anthony P.; Kuc, Rhoda E.; Ashby, Michael J.; Patt, William C.; Doherty, Annette M.
CORPORATE SOURCE: Addenbrooke's Hospital, University of Cambridge, Cambridge, CB2 2QQ, UK
SOURCE: British Journal of Pharmacology (1998), 123(2), 223-230
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Stockton Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have synthesized a new low mol. weight, non-peptide radioligand, [125I]-PD164333, an analog of the orally active butenolide antagonists of the endothelin ETA receptor. Anal. of saturation binding assays demonstrated that [125I]-PD164333 bound with high affinity to a single population of receptors,. In each case Hill slopes were close to unity. In kinetic expts., the binding of [125I]-PD164333 to ETA receptors in sections of heart was time-dependent and rapid at 23°C. The data were fitted to a one site model, with an association rate constant K1 of 2.66 ± 0.213 x 108 M-1 min-1, and a half-time for association of 11 min. The binding was reversible at 23°C: anal. of the data indicated [125I]-PD164333 dissociated from a single site, with a dissociation rate constant of 0.0031 ± 0.0004 min-1, a half-time for dissociation of 216 min and a KD calculated from these kinetic data of 0.01 nM. Unlabeled PD164333 inhibited the binding of [125I]-ET-1 to left ventricle (which expresses both subtypes) in a biphasic manner with a KDETA of 0.99 ± 0.32 nM and KDETB of 2.41 ± 0.22 μM, giving a selectivity of 2500 fold. ETA-selective ligands competed monophasically for [125I]-PD164333 binding in left ventricle, a one site fit was preferred to a two site model giving similar nanomolar affinities: BQ123, KD = 3.93 + 0.18 nM; FR139317 KD = 3.53 ± 0.69 nM. In contrast, the ETB selective agonists, BQ3020 and sarafotoxin S6c (1 μM) did not inhibit binding. In human isolated saphenous vein, unlabeled PD164333 was a functional antagonist, producing parallel rightward shifts of the endothelin-1 (ET-1) concentration-response curve (pA2 = 8.84) and a slope of unity. In the human brain, autoradiog. revealed high levels of [125I]-PD164333 binding to the pial arteries of the cerebral cortex and to the numerous smaller intercerebral vessels penetrating the underlying gray and white matter. Conduit and resistance vessels contributing to the control of blood pressure from the heart, kidney, lungs and adrenal also displayed high densities of binding. In diseased vessels, binding of [125I]-PD164333 was confined to the medial layer of both coronary arteries with advanced atherosclerotic lesions or occluded saphenous vein grafts. In contrast, little or no binding was detected in the proliferated smooth muscle of the intimal layer or occluded lesion. These results show [125I]-PD164333 is a specific, high affinity, reversible non-peptide radioligand for human ETA receptors, which will facilitate the further characterization of this subtype, in vitro and in vivo.

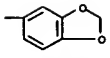
IT 204273-83-6, [125I]-PD 164333 204326-22-7, PD 164333
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(([125I]-PD-164333 ETA selective non-peptide radiolabeled antagonist in normal and diseased human tissues)

RN 204273-83-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-[4-[[2-[4-hydroxy-3-(iodo-125I)phenyl]ethyl]amino]-4-oxobutoxy]-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

PAGE 1-A



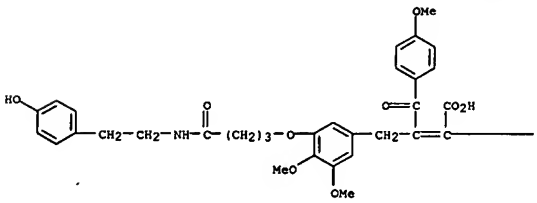
PAGE 1-B



RN 204326-22-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-[4-[[2-(4-hydroxyphenyl)ethyl]amino]-4-oxobutoxy]-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 84 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



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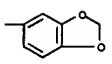
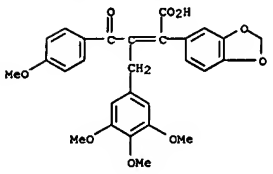


REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 85 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:72651 CAPLUS
DOCUMENT NUMBER: 128:200558
TITLE: Design and pharmacological evaluation of a series of non-peptide endothelin ETA selective and ETA/ETB receptor antagonists
AUTHOR(S): Doherty, A.; Patt, W.; Reisdorph, B.; Repine, J.; Walker, D.; Flynn, M.; Welch, K.; Reynolds, E.; Haleen, S.
CORPORATE SOURCE: Parke-Davis Pharmaceutical Research, Division of Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Medicinal Chemistry: Today and Tomorrow, Proceedings of the AFMC International Medicinal Chemistry Symposium, Tokyo, Sept. 3-8, 1995 (1997), Meeting Date
1995, 255-261. Editor(s): Yamazaki, Mikio. Blackwell: Oxford, UK.
CODEN: 65ONAG
DOCUMENT TYPE: Conference
LANGUAGE: English
AB This report will describe the design and pharmacol. evaluation of both ETA
selective and ETA/ETB antagonists from the PD 155080 and PD 156707 series of orally active non-peptide ETA selective antagonists. Modification of the substituents around the butenolide ring has lead to compound with differing selectivity for human ETA and ETB receptors. For example, several analogs of the subnanomolar affinity ETA selective antagonist PD 156707 have been designed as either potent ETA or balanced ETA/ETB antagonists. In this series the di-allyloxy analog (PD 161867) of PD 156707 is 7500-fold selective for the human ETA receptor. ETA/ETB antagonists from this series include PD 160874, 162073 and 160672. For example, PD 160874 is a competitive inhibitor of [125I]ET-1 and {125I]ET-3
binding to human cloned ETA and ETB receptors with IC50's of 3.5 nM (ETA) and 8.9 nM (ETB) resp. while PD 162073 exhibits and pharmacol. evaluation of the non-peptide orally active PD 156707 series of ET antagonists where the selectivity ratios for ETA and ETB receptors have been varied from >2000 to 20-fold will be described.
IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); PRP (Properties); BIOL (Biological study)
(design and pharmacol. evaluation of a series of non-peptide endothelin
ETA selective and ETA/ETB receptor antagonists (PD 156707 analogs))
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX
NAME)

L4 ANSWER 85 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
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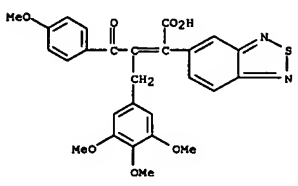
L4 ANSWER 86 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:48487 CAPLUS
DOCUMENT NUMBER: 128:188293
TITLE: 2. Endothelin antagonists: evaluation of 2,1,3-benzothiadiazole as a methylenedioxyphenyl bioisoster
AUTHOR(S): Mederski, Werner W. K. R.; Osswald, Mathias; Dorsch, Dieter; Anzali, Soheila; Christadler, Maria; Schmitges, Claus-Jochen; Wilm, Claudia
CORPORATE SOURCE: Pharmaceutical Research, Merck KGaA, Darmstadt, 64271,
Germany
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998), 8(1),
17-22
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The methylenedioxyphenyl group is present in a number of endothelin receptor
antagonists thus far reported. By a Kohonen neural network we discovered with a benzothiadiazole a bioisosteric replacement instead. This group should be devoid of the neg. metabolic interactions with cytochrome P 450 ascribed to methylenedioxyphenyl in vivo. The synthesis of a potent benzothiadiazole analog EMD 122801 together with in vitro studies of different methylenedioxyphenyl, benzothiadiazole and benzofurazan derivs. is described.
IT 195505-82-9P, EMD 122801
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and structure activity relations of benzothiadiazole endothelin
antagonists)
RN 195505-82-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX
NAME)



● Na

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 86 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

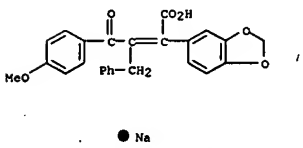
L4 ANSWER 87 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:12635 CAPLUS
DOCUMENT NUMBER: 128:100698
TITLE: Role of endothelin in hypertension of experimental chronic renal failure
AUTHOR(S): Potter, Gregg S.; Johnson, Ron J.; Fink, Gregory D.
CORPORATE SOURCE: Department of Pharmacology and Toxicology, Michigan State University, East Lansing, MI, 48824-1317, USA
SOURCE: Hypertension (Dallas) (1997), 30(6), 1578-1584
CODEN: HPRTDN; ISSN: 0194-911X
PUBLISHER: American Heart Association
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Surgical ablation of renal mass leads to a reduction in kidney function and commonly to the development of hypertension and chronic renal failure (CRF) in rats. The objective of this study was to determine whether endothelin (ET)-1 is involved in the maintenance of the hypertension that accompanies loss of renal mass. First, the authors demonstrated the antihypertensive efficacy of PD 155080, a selective, orally active ETA receptor antagonist, in a group of rats made hypertensive by continuous i.v. infusion of ET-1 (2.5 pmol/kg/min) for 7 days. ET-1 produced a sustained hypertension and PD 155080 [56.4 μmol/kg (25mg/kg) BID PO] normalized blood pressure (BP) during the 5 days of drug administration. In a second experiment, Sprague-Dawley rats underwent a 5/6 reduction in renal mass (RRM); 4 wk later, PD 155080 administered for 7 days resulted in a sustained reduction in BP. Sham-operated rats also showed a slight hypotensive response to PD 155080 administration. Plasma urea nitrogen, plasma creatinine, urinary protein excretion, and creatinine clearance were not altered by PD 155080 administration in RRM or sham rats. In a third experiment, the authors investigated the contribution of the renin-angiotensin system to BP control in RRM rats given PD 155080. In these rats, PD 155080 reduced BP during 5 treatment days, and this antihypertensive effect was not altered by co-administration of the angiotensin-converting enzyme inhibitor enalapril in the drinking water [508 μmol/L (250 mg/L)]. Thus, (1) ET-1 plays a role in established RRM hypertension through activation of the ETA receptor subtype, (2) lowering blood pressure with PD 155080 in RRM rats does not adversely affect renal function, and (3) the antihypertensive effect of ETA receptor antagonism is not opposed by the renin-angiotensin system.

IT 162412-71-7, PD 155080
RL: BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(role of endothelin in hypertension of chronic renal failure mediated by excision-induced renal mass reduction)

RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 87 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



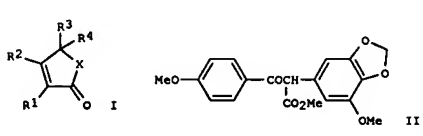
● Na

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:780649 CAPLUS
DOCUMENT NUMBER: 128:48214
TITLE: Preparation of 3,5-diphenyl-2(5H)-furanone derivatives as nonpeptide endothelin I antagonists
INVENTOR(S): Berryman, Kent Alan; Doherty, Annette Marian; Edmunds, Jeremy John; Patt, William Chester; Plummer, Mark Stephen; Repine, Joseph Thomas
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: U.S., 120 pp., Cont.-in-part of U.S. Ser. No. 278,882, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5691373	A	19971125	US 1995-384083	19950206
CA 2165567	A1	19950223	CA 1994-2165567	19940809
HU 74179	A2	19961128	HU 1996-365	19940809
ZA 9406265	A	19960219	ZA 1994-6265	19940818
US 6017916	A	20000125	US 1997-787423	19970122
PRIORITY APPLN. INFO.:			US 1993-109751	B2 19930819
			US 1994-217578	B2 19940324
			US 1994-278882	B2 19940726
			US 1995-384083	A3 19950206

OTHER SOURCE(S): MARPAT 128:48214
GI



AB Novel nonpeptide antagonists of endothelin I represented by formula [I; R1 = (un)substituted C3-12 cycloalkyl, Ph substituted with 1-5 substituents, naphthyl or heteroaryl optionally substituted with 1-5 substituents; R2 = C1-12 linear or branched alkyl, C3-12 linear or branched cycloalkyl, aryl optionally substituted with 1-5 substituents, heteroaryl optionally substituted with 1-3 substituents; R3 = (un)substituted C1-12 linear or branched alkyl, (un)substituted C3-12 cycloalkyl, aryl optionally substituted with 1-5 substituents, heteroaryl optionally substituted with 1-3 substituents; R4 = OH, OR5, (CH2)nOR5; wherein R5 = (un)substituted

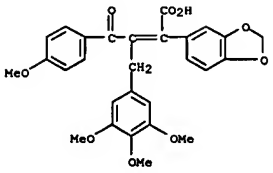
L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

C1-7 alkyl; X = O, S] or tautomeric open chain keto-acids forms thereof or pharmaceutically acceptable salt thereof are prepd. Also described are pharmaceutical compns. of the above compds., which are useful in treating elevated levels of endothelin, acute and chronic renal failure, hypertension, myocardial infarction, myocardial ischemia, cerebral vasospasm, cerebral ischemia, cerebral infarction, cirrhosis, septic shock, congestive heart failure, endotoxic shock, subarachnoid hemorrhage, arrhythmia, asthma, preeclampsia, atherosclerotic disorders including Raynaud's disease and restenosis, angina, cancer, pulmonary hypertension, ischemic disease, gastric mucosal damage, hemorrhagic shock, ischemic bowel disease, stroke, benign prostatic hyperplasia (BPH), and diabetes. Thus, Me 2-benzoyl-2-phenylacetate deriv. (II) and 3,4,5-trimethoxybenzladehyde were refluxed in the presence of NaOMe in MeOH for 18 h and the soln. was treated with AcOH and refluxed an addnl. 72 h, followed by sapon. of the product with 1N aq. NaOH and acidification to give 28% I (X = O, R1 = Q, R2 = 3,4,5-trimethoxyphenyl, R3 = 4-methoxyphenyl, R4 = OH). The latter compd. in vitro showed an antagonism of endothelin I-stimulated vasoconstriction in the rabbit femoral artery and sarafotoxin 6c-stimulated vasoconstriction in the rabbit pulmonary artery with pA2 values of 0.00025 and 0.34, resp.

IT 162412-70-6P 162412-71-7P 169804-10-8P
169804-12-0P 169804-14-2P 169804-77-7P
169805-53-2P 169805-54-3P 169805-58-7P
169805-59-8P 169805-68-9P 169805-69-0P
169805-70-3P 169805-71-4P 169805-72-5P
169805-73-6P 169805-80-5P 169805-82-7P
169805-89-4P 169806-08-0P 199738-46-0P
199741-20-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diphenylfuranone derivs. as nonpeptide endothelin I antagonists for disease treatment)

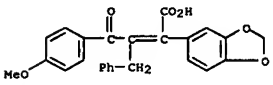
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-(2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



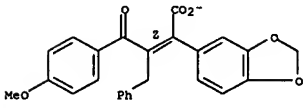
● Na

RN 169804-10-8 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 169804-09-5
CMF C25 H19 O6

Double bond geometry as shown.



CM 2

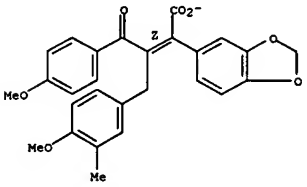
CRN 62-49-7
CMF C5 H14 N O

RN 169804-12-0 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[1-[(4-methoxy-3-methylphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

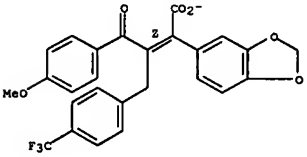
CRN 169804-11-9
CMF C27 H23 O7

Double bond geometry as shown.



CM 2

CRN 62-49-7
CMF C5 H14 N O



CM 2

CRN 62-49-7
CMF C5 H14 N O

RN 169804-14-2 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[2-(4-methoxyphenyl)-2-oxo-1-[[4-(trifluoromethyl)phenyl]methyl]ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 169804-13-1
CMF C26 H18 F3 O6

Double bond geometry as shown.

CM 2

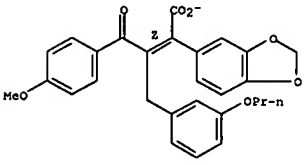
CRN 62-49-7
CMF C5 H14 N O

RN 169804-77-7 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[2-(4-methoxyphenyl)-2-oxo-1-[(3-propoxyphenyl)methyl]ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

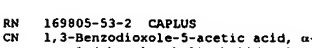
CRN 169804-76-6
CMF C28 H25 O7

Double bond geometry as shown.

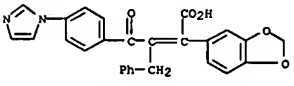


CM 2

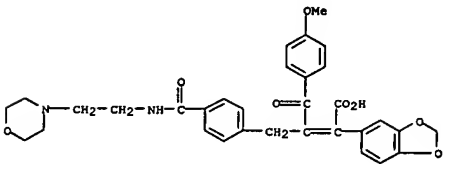
CRN 62-49-7
CMF C5 H14 N O



RN 169805-53-2 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-[4-(1H-imidazol-1-yl)phenyl]-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)

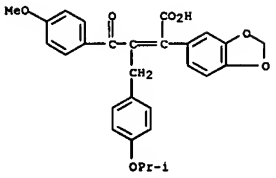


RN 169805-54-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[[4-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]phenyl]methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



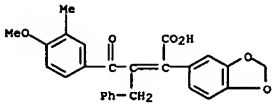
RN 169805-58-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[[4-(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INDEX NAME)



● Na

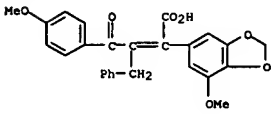
RN 169805-59-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

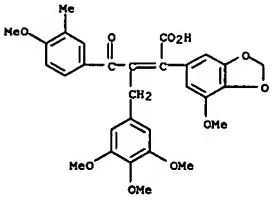
RN 169805-68-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[4-(acetylamino)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, monopotassium salt (9CI) (CA INDEX
NAME)

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

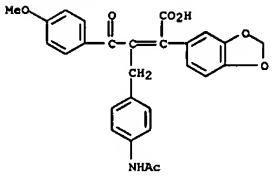
RN 169805-71-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium
salt (9CI) (CA INDEX NAME)



● Na

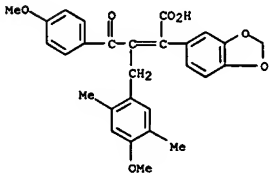
RN 169805-72-5 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● K

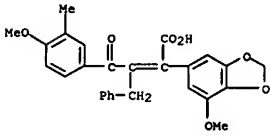
RN 169805-69-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(4-methoxy-2,5-dimethylphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

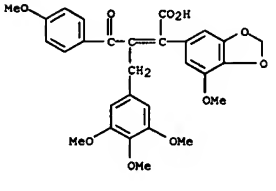
RN 169805-70-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

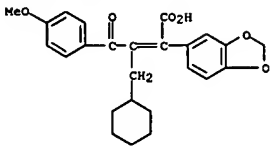
RN 169805-73-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA
INDEX NAME)



● Na

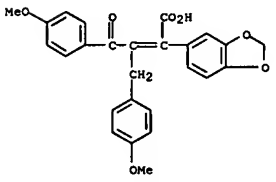
RN 169805-80-5 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-(cyclohexylmethyl)-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

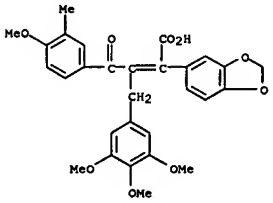
RN 169805-82-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-methoxyphenyl)methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

RN 169805-89-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

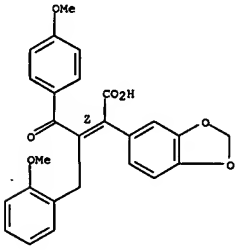
L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 169806-08-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(2-methoxyphenyl)methyl]-2-oxoethylidene]-, sodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● Na

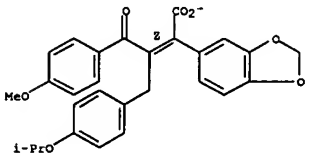
RN 199738-46-0 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[2-(4-methoxyphenyl)-1-[[4-(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 199738-45-9
CMF C28 H25 O7

Double bond geometry as shown.

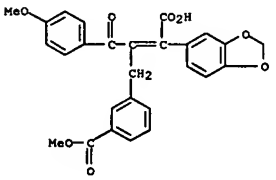


CM 2

CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N-CH_2-CH_2-OH$

RN 199741-20-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-(methoxycarbonyl)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, potassium salt (9CI) (CA INDEX NAME)

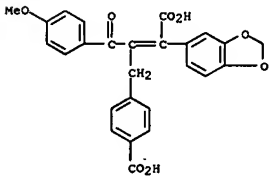


● K

IT 169805-00-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of diphenylfuranone derivs. as nonpeptide endothelin I antagonists for disease treatment)

L4 ANSWER 88 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 169805-00-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(4-carboxyphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, disodium salt (9CI) (CA INDEX NAME)



●2 Na

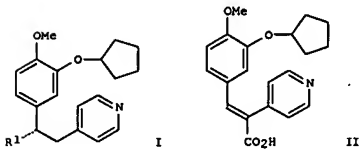
L4 ANSWER 89 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:746033 CAPLUS
DOCUMENT NUMBER: 128:22818
TITLE: Preparation of chiral diarylethylpyridine phosphodiesterase IV inhibitors
INVENTOR(S): Choi, Woo-Baeg; Churchill, Hywyn R. O.; Lynch, Joseph E.; Reider, Paul J.; Volante, Ralph P.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9742172	A1	19971113	WO 1997-US7457	19970505
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2253279	A1	19971113	CA 1997-2253279	19970505
AU 9728252	A	19971126	AU 1997-28252	19970505
AU 707289	B2	19990708		
EP 912517	A1	19990506	EP 1997-922629	19970505
EP 912517	B1	20001025		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2000510120	T	20000808	JP 1997-540058	19970505
AT 197148	T	20001115	AT 1997-922629	19970505
ES 2151728	T3	20010101	ES 1997-922629	19970505
PT 912517	T	20010330	PT 1997-922629	19970505
TW 418192	B	20010111	TW 1997-86107985	19970610
GR 3034674	T3	20010131	GR 2000-402338	20001026

PRIORITY APPLN. INFO.: US 1996-16839P P 19960508
GB 1996-14329 A 19960708
US 1996-16839 P 19960508
WO 1997-US7457 W 19970505

OTHER SOURCE(S): MARPAT 128:22818
GI

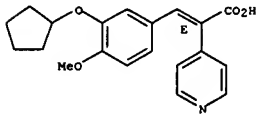
L4 ANSWER 89 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I II

AB Title compds. [I; R1 = (substituted) Ph], were prepared starting by reaction of unsatd. acid (II) with (1R,2S)-cis-aminoindanol to give the corresponding amide, which was converted to the acetonide derivative followed by conjugate addition of an aryllithium, aryl Grignard, or aryl cuprate, and base hydrolysis. I (R = Ph) was prepared having an R:S ratio of 99.73:0.27.
IT 199331-21-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral diarylethylpyridine phosphodiesterase IV inhibitors)
RN 199331-21-0 CAPLUS
CN 4-Pyridineacetic acid, α-[(3-(cyclopentyloxy)-4-methoxyphenyl]methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:684399 CAPLUS
DOCUMENT NUMBER: 127:346381
TITLE: Preparation of heterocyclyl ketoacids as endothelin antagonists
INVENTOR(S): Cheng, Xue-Min; Doherty, Annette Marian; Hurley, Timothy Robert; Lovdahl, Michael James; Patt, William Chester; Repine, Joseph Thomas
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9737987	A1	19971016	WO 1997-US3959	19970312
W: AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9725292	A	19971029	AU 1997-25292	19970312
ZA 9703024	A	19971104	ZA 1997-3024	19970409
US 6043241	A	20000328	US 1998-117575	19980731

PRIORITY APPLN. INFO.: US 1996-15269P P 19960410
WO 1997-US3959 W 19970312

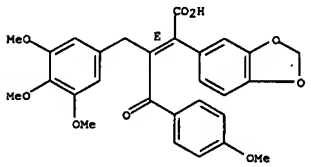
OTHER SOURCE(S): MARPAT 127:346381
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; R1 = H, alkyl, alkoxy, etc.; R2 = H, alkoxy; R3 = H, alkyl; alkoxy; R2R3 = OCH2O, OCH2CH2O; R4 = H, alkoxy; R5 = H, alkoxy, O-allyl; R6 = H, alkoxy, O-allyl; R7 = H, alkoxy, NH2, etc.; R5R6 = OCH2O; R6R7 = OCH2O; R8 = H, alkoxy; R9 = H, alkyl, alkoxy; R10 = alkoxy, amino; R9R10 = OCH2O; R11 = H, alkyl, alkoxy; R12 = H, alkoxy], novel nonpeptide antagonists of endothelin I which are useful in treating acute respiratory distress syndrome (ARDS), atherosclerosis, restenosis, Raynaud's phenomenon, chronic obstructive pulmonary diseases, mild or severe congestive heart failure, cerebral ischemia, cerebral infarction, embolic stroke, cerebral vasospasm, glaucoma, subarachnoid hemorrhage, hemorrhagic stroke, diabetes, gastric ulceration and mucosal damage, ischemic bowel disease, Crohn's disease, essential or malignant hypertension, pulmonary hypertension, pulmonary hypertension after bypass, male penile erectile dysfunction, cancer, especially malignant hemangioendothelioma or prostate cancer, myocardial infarction or ischemia, acute or chronic renal failure

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
renal ischemia, radiocontrast-induced nephrotoxicity, endotoxic, septic, hemorrhagic shock, angina, preeclampsia, asthma, arrhythmias, benign prostatic hyperplasia, and elevated levels or endothelin, were prepd. by reacting an α-hydroxy butenolide II with one or more equiv. of a suitable base, and exposing the above mentioned soln. to an UV light. Thus, compd. (E)-I [R1 = H; R2R3 = OCH2O; R4 = R8 = H; R5-R7 = MeO; R9, R11, R12 = H; R10 = MeO] showed IC50 of 65 nM against HERBA-A (Ltk- cells expressing human ETAR).
IT 198288-36-7P 198288-38-9P 198288-40-3P
198288-41-4P 198288-42-5P 198288-43-6P
198288-44-7P 198288-45-8P 198288-46-9P
198288-47-0P 198288-48-1P 198288-49-2P
198288-50-5P 198288-51-6P 198288-52-7P
198288-53-8P 198288-54-9P 198288-55-0P
198288-56-1P 198288-60-7P 198288-61-8P
198288-62-9P 198288-63-0P 198288-64-1P
198288-65-2P 198288-66-3P 198288-67-4P
198288-68-5P 198288-69-6P 198288-70-9P
198288-75-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyl ketoacids as endothelin antagonists)
RN 198288-36-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

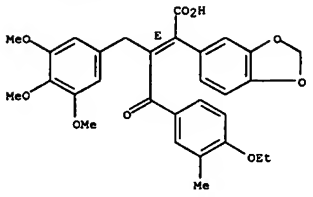
Double bond geometry as shown.



RN 198288-38-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-ethoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

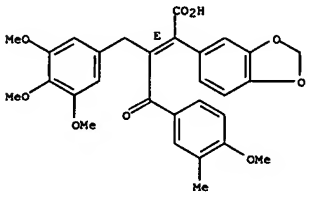
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 198288-40-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

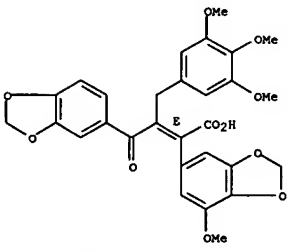
Double bond geometry as shown.



RN 198288-41-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

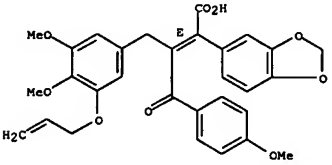
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



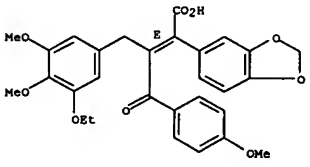
RN 198288-44-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-(2-propenyloxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

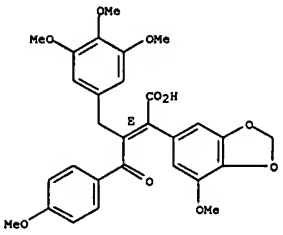


RN 198288-45-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(3-ethoxy-4,5-dimethoxyphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

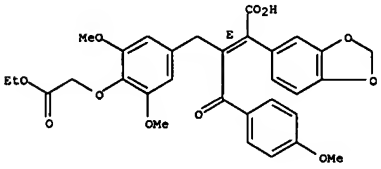


L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 198288-42-5 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[4-(2-ethoxy-2-oxoethoxy)-3,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



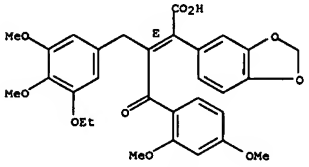
RN 198288-43-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(1,3-benzodioxol-5-yl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-7-methoxy-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

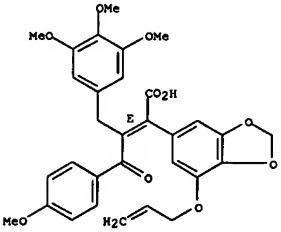
RN 198288-46-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(2,4-dimethoxyphenyl)-1-[(3-ethoxy-4,5-dimethoxyphenyl)methyl]-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198288-47-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-7-(2-propenyloxy)-, (E)- (9CI)
(CA INDEX NAME)

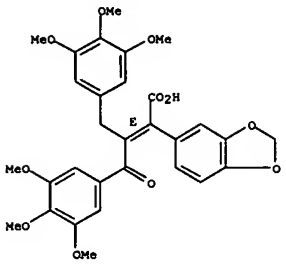
Double bond geometry as shown.



RN 198288-48-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-oxo-2-(3,4,5-trimethoxyphenyl)-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

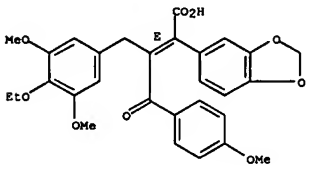
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 198288-49-2 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(4-ethoxy-3,5-dimethoxyphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

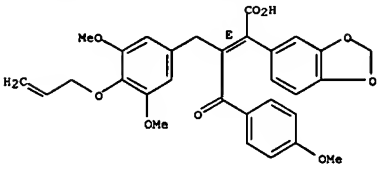
Double bond geometry as shown.



RN 198288-50-5 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,5-dimethoxy-4-(2-propenyloxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

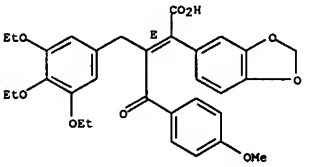
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



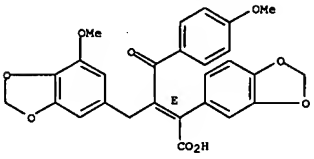
RN 198288-51-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-triethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198288-52-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(7-methoxy-1,3-benzodioxol-5-yl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

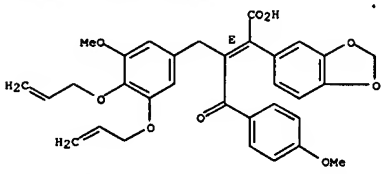
Double bond geometry as shown.



RN 198288-53-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-methoxy-4,5-bis(2-

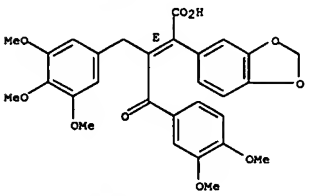
L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
propenyloxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198288-54-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(3,4-dimethoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

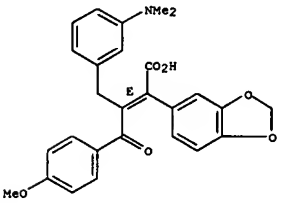
Double bond geometry as shown.



RN 198288-55-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-(dimethylamino)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

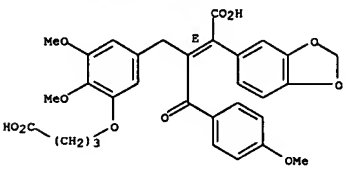
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



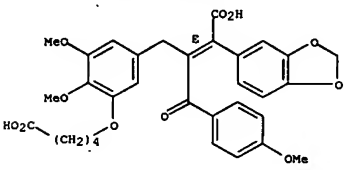
RN 198288-56-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-(3-carboxypropoxy)-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198288-60-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-(4-carboxybutoxy)-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

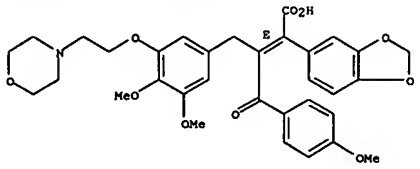
Double bond geometry as shown.



RN 198288-61-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-[2-(4-

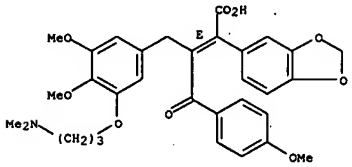
L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
morpholinyl)ethoxy]phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198288-62-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-[3-(dimethylamino)propoxy]-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

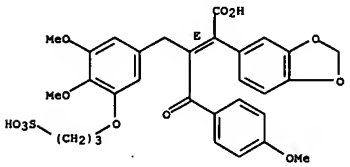
Double bond geometry as shown.



RN 198288-63-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-(3-sulfopropoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

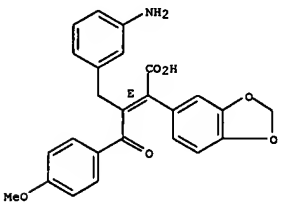
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 198288-64-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(3-aminophenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

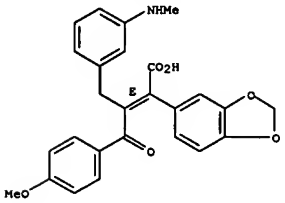
Double bond geometry as shown.



RN 198288-65-2 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[[3-(methylamino)phenyl]methyl]-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

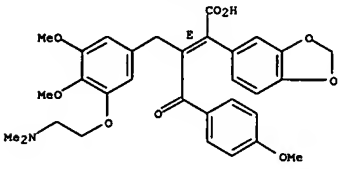
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



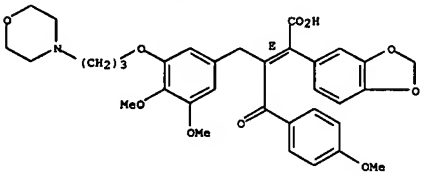
RN 198288-66-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-[2-(dimethylamino)ethoxy]-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198288-67-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-[3-(4-morpholinyl)propoxy]phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

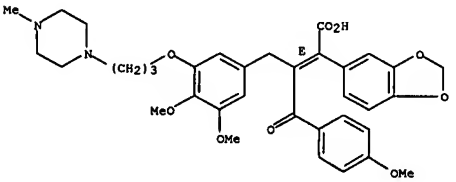
Double bond geometry as shown.



RN 198288-68-5 CAPLUS

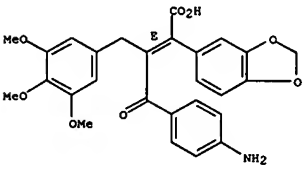
L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-[3-(4-methyl-1-piperazinyl)propoxy]phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198288-69-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-aminophenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

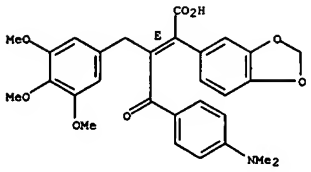
Double bond geometry as shown.



RN 198288-70-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-[4-(dimethylamino)phenyl]-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, (E)- (9CI) (CA INDEX NAME)

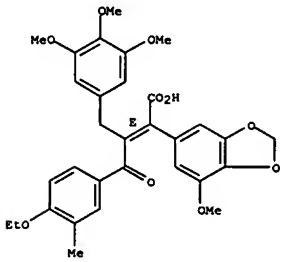
Double bond geometry as shown.

L4 ANSWER 90 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 198288-75-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-ethoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-7-methoxy-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

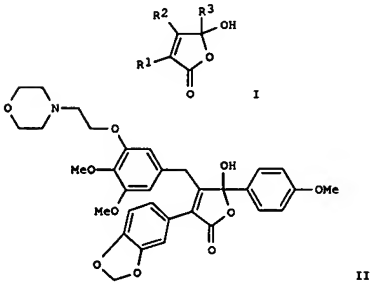


L4 ANSWER 91 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:684397 CAPLUS
DOCUMENT NUMBER: 127:346287
TITLE: Nonpeptide endothelin antagonists with increased water solubility
INVENTOR(S): Cheng, Xue-Min; Doherty, Annette Marian; Patt, William
Chester; Repine, Joseph Thomas
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: PCT Int. Appl., 106 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9737985	A1	19971016	WO 1997-US3929	19970312
W: AL, AU, BA, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9720778	A	19971029	AU 1997-20778	19970312
ZA 9703026	A	19971104	ZA 1997-3026	19970409
US 6297274	B1	20011002	US 1998-117667	19980804
PRIORITY APPLN. INFO.:			US 1996-15242P P	19960410
			WO 1997-US3929 W	19970312

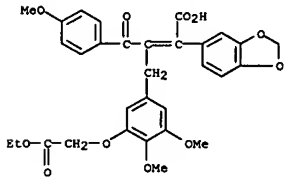
OTHER SOURCE(S): MARPAT 127:346287
GI

L4 ANSWER 91 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

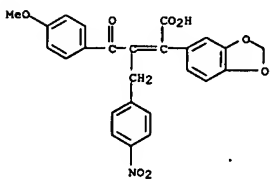


AB Novel nonpeptide antagonists of endothelin are described, specifically the
butenolides I [R1 = (un)substituted cycloalkyl, Ph, naphthyl, or heteroaryl; R2 = (un)substituted alkyl, cycloalkyl, aryl, or heteroaryl; R3 = (un)substituted alkyl, cycloalkyl, aryl, or heteroaryl; mol. bears at
least 1 water solubility-enhancing substituent, and up to 4 total aqueous solubility
groups; provided that when R2 = substituted alkyl, the substituent is not O located alpha to the furanone ring]. Also disclosed are methods for the
preparation of I, and their pharmaceutical compns., which are useful in treating atherosclerosis, restenosis, Raynaud's phenomenon, mild or severe
congestive heart failure, cerebral ischemia, cerebral infarction, embolic stroke, cerebral vasospasm, glaucoma, subarachnoid hemorrhage, hemorrhagic
stroke, diabetes, gastric ulceration and mucosal damage, ischemic bowel disease, Crohn's disease, male penile erectile dysfunction, essential or malignant hypertension, pulmonary hypertension, pulmonary hypertension after bypass, cancer, especially malignant hemangioendothelioma or prostate
cancer, myocardial infarction or ischemia, acute or chronic renal failure,
renal ischemia, radiocontrast-induced nephrotoxicity, endotoxic, septic, or hemorrhagic shock, angina, preeclampsia, asthma, arrhythmias, benign prostatic hyperplasia, and elevated levels of endothelin. Example preps.
of 38 compds. and/or their salts, and 22 intermediates, are described. For instance, cyclocondensation of 2-benzo[1,3]dioxol-5-yl-4-(4-methoxyphenyl)-4-oxobutyric acid Me ester with 3-[2-(N-morpholinyl)ethoxy]-
4,5-dimethoxybenzaldehyde in the presence of NaOMe, followed by treatment with AcOH, gave title compound II. In assays against human cloned receptors

L4 ANSWER 91 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
in vitro, II had IC50 values of 0.3 nM at ETA receptors and 2300 nM at ETB
receptors. Aq. soly. of I was excellent, with three representative compds. having soly. values of at least 25-80 mg/mL.
IT 198271-31-7P 198271-49-7P 198271-50-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of furanone derivs. as nonpeptide endothelin
antagonists with increased aqueous solubility)
RN 198271-31-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-(2-ethoxy-2-oxoethoxy)-4,5-dimethoxyphenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

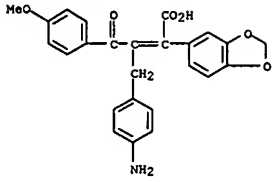


RN 198271-49-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-nitrophenyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)

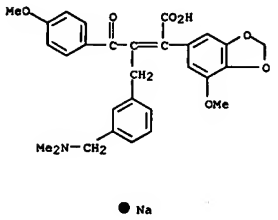


RN 198271-50-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(4-aminophenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 91 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 198271-26-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of furanone derivs. as nonpeptide endothelin antagonists with increased aqueous solubility)
RN 198271-26-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[3-[(dimethylamino)methyl]phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-7-methoxy-, sodium salt (9CI) (CA INDEX NAME)



● Na

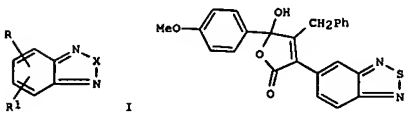
L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:579706 CAPLUS
DOCUMENT NUMBER: 127:248116
TITLE: 2,1,3-benzothia(oxa)diazole derivatives having an endothelin receptor antagonistic effect
INVENTOR(S): Dorsch, Dieter; Osswald, Mathias; Mederski, Werner; Wilm, Claudia; Schmitges, Claus; Christadler, Maria; Anzali, Soheila
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany; Osswald, Mathias; Mederski, Werner; Wilm, Claudia; Schmitges, Claus; Christadler, Maria; Anzali, Soheila
SOURCE: PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9730982	A1	19970828	WO 1997-EP818	19970220
W: AU, BR, CA, CN, CZ, HU, JP, KR, LT, LV, MX, NO, PL, RU, SI, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19607096	A1	19970828	DE 1996-19607096	19960224
ZA 9701466	A	19970828	ZA 1997-1466	19970220
AU 9718757	A	19970910	AU 1997-18757	19970220
AU 721203	B2	20000629		
EP 882030	A1	19981209	EP 1997-905065	19970220
EP 882030	B1	20010912		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI				
CN 1216540	A	19990512	CN 1997-193959	19970220
CN 1072660	B	20011010		
AT 205486	T	20010915	AT 1997-905065	19970220
RU 2175320	C2	20011027	RU 1998-117806	19970220
ES 2164328	T3	20020216	ES 1997-905065	19970220
PT 882030	T	20020328	PT 1997-905065	19970220
US 6017939	A	20000125	US 1998-142408	19981112

PRIORITY APPLN. INFO.: DE 1996-19607096 A 19960224
WO 1997-EP818 W 19970220

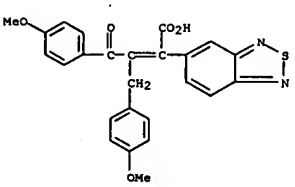
OTHER SOURCE(S): MARPAT 127:248116
GI

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



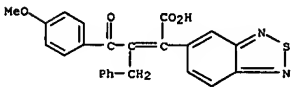
I II

AB Title compds. I [R = C(CO2H):C(COR3)(CH2)nR2, COC[(CH2)nR2]:CR4CO2H, (CH2)nC(COR3):CR4CO2H; X = O, S; R1 = H, halogen, (un)substituted alkoxy, alkyl, NO2, NH2, acylamino, SO2NH2, SO3H, CHO; R2-R4 = (un)substituted Ph, heterocyclic; n = 0-2] were prepared as endothelin receptor antagonists (no data). Thus, 3,4-(H2N)2C6H3CH2CO2Et was treated with thionylaniline to give Et 2-(2,1,3-benzothiadiazol-5-yl)acetate which was treated with 4-MeOC6H4COCH2Br and then with benzaldehyde to give the benzothiadiazole II.
IT 195505-54-5P 195505-81-8P 195505-82-9P
195505-83-0P 195505-84-1P 195505-86-3P
195505-87-4P 195505-88-5P 195505-94-3P
195506-92-4P 195506-93-5P 195506-94-6P
195506-95-7P 195506-96-8P 195506-97-9P
195506-98-0P 195507-00-7P 195507-01-8P
195507-02-9P 195507-03-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzothiadiazole derivs. as endothelin receptor antagonists)
RN 195505-54-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-methoxyphenyl)methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



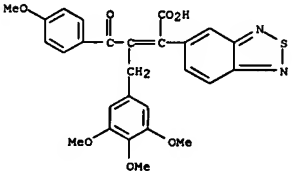
RN 195505-81-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

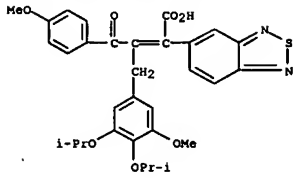
RN 195505-82-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

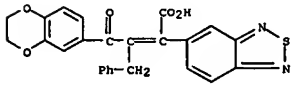
RN 195505-83-0 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3-methoxy-4,5-bis(1-methylethoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

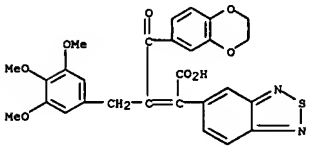
RN 195505-84-1 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

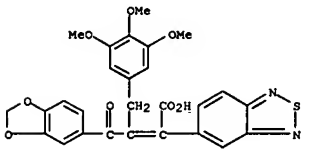
RN 195505-86-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

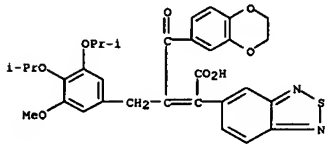
RN 195505-87-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(1,3-benzodioxol-5-yl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

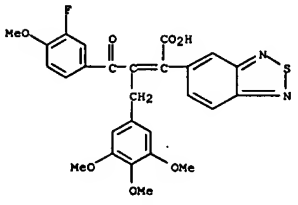
RN 195505-88-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-[[3-methoxy-4,5-bis(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

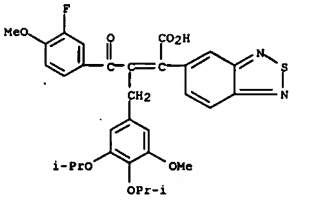
RN 195505-94-3 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

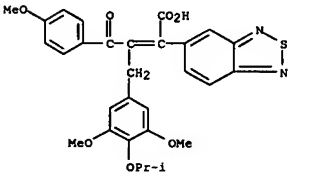
RN 195506-92-4 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-1-[[3-methoxy-4,5-bis(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

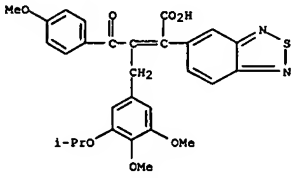
RN 195506-93-5 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3,5-dimethoxy-4-(1-methylethoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

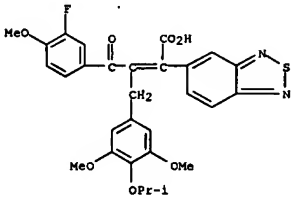
RN 195506-94-6 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3,4-dimethoxy-5-(1-methylethoxy)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

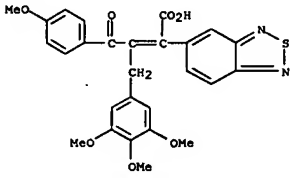
RN 195506-95-7 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[3,5-dimethoxy-4-(1-methylethoxy)phenyl]methyl]-2-(3-fluoro-4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

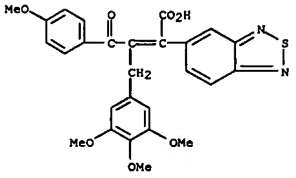
RN 195506-96-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, potassium salt (9CI) (CA INDEX NAME)

L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



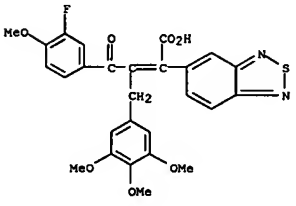
● K

RN 195506-97-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

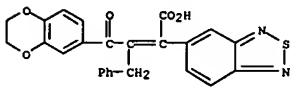


RN 195506-98-0 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]- (9CI) (CA INDEX NAME)

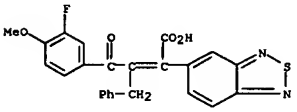
L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 195507-00-7 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)

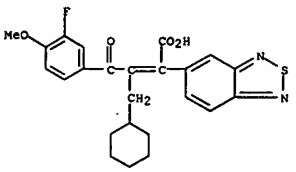


RN 195507-01-8 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[2-(3-fluoro-4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)

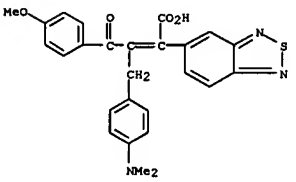


RN 195507-02-9 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-(cyclohexylmethyl)-2-(3-fluoro-4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)

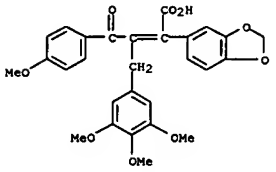
L4 ANSWER 92 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 195507-03-0 CAPLUS
CN 2,1,3-Benzothiadiazole-5-acetic acid, α-[1-[[4-(dimethylamino)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]- (9CI) (CA INDEX NAME)



L4 ANSWER 93 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:559747 CAPLUS
DOCUMENT NUMBER: 127:243116
TITLE: Endothelin antagonists in focal cerebral ischemia
AUTHOR(S): Mcculloch, J.; Takasago, T.; Galbraith, S.; Graham, D.
I.; Patel, T. R.
CORPORATE SOURCE: Wellcome Surgical Institute & Hugh Fraser Neuroscience
Labs., University of Glasgow, Glasgow, G61 1QH, UK
SOURCE: Pharmacology of Cerebral Ischemia 1996, [International
Symposium on Pharmacology of Cerebral Ischemia], 6th, Marburg, July 21-24, 1996 (1996), 619-624.
Editor(s):
Krieglstein, Josef. Medpharm Scientific Publishers: Stuttgart, Germany.
CODEN: 64YHA7
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The present investigation indicated that, in cats and rats, blockage of ETA receptors with the antagonist PD 156707 reduced the volume of ischemic
brain damage after permanent middle cerebral artery occlusion.
IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(endothelin antagonists for treatment of focal cerebral ischemia)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX
NAME)

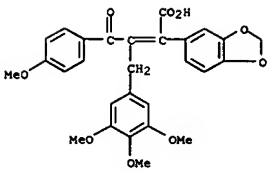


● Na

L4 ANSWER 93 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 94 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:318383 CAPLUS
DOCUMENT NUMBER: 127:13231
TITLE: Endothelin receptor antagonists: effect of serum albumin on potency and comparison of pharmacological characteristics
AUTHOR(S): Wu-Wong, Jinshyun R.; Dixon, Douglas B.; Chiou, William J.; Opgenorth, Terry J.
CORPORATE SOURCE: Pharmaceutical Products Division, Abbott Laboratories,
Abbott Park, IL, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1997), 281(2), 791-798
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Endothelins (ETs) are 21-amino acid peptides that bind to membrane receptors to initiate pathophysiol. effects. Two types of ET receptors, ETA and ET, have been identified. Various ET receptor antagonists are being developed as therapeutic agents. This report examines the effects of bovine serum albumin (BSA) on the potency of ET receptor antagonists and compares five ET receptor antagonists. Competition studies show that in the absence of BSA, A-127722 and L-749329 inhibited ET-1 binding to ETA
receptor with the same IC50 value of 0.09 nM. Addition of increasing concns.
of BSA incrementally decreased the potency of the antagonists: in the presence of 5% BSA, the IC50 values increased to 4.3 and 820 nM, resp. Similarly, addition of BSA decreased the potency of antagonists in inhibiting
ET-1-stimulated phosphatidylinositol hydrolysis. These results suggest that serum albumin has profound effects on the potencies of ET receptor antagonists. FR139317, PD-156707, L-749329, Ro-47-0203 and A-127722 were then selected for direct comparison under identical exptl. conditions with
0.2% BSA. The potency of antagonists was assessed by binding studies for the determination of IC50 and Ki values and by ET-1-stimulated phosphatidylinositol hydrolysis and arachidonic acid release for the determination
of IC50 and pA2 values. All five antagonists inhibited ET binding and the
biol. effects exerted by ET in a competitive mode. The Ki values for A-127722, PD-156707, FR139317, Ro-47-0203 and L-749329 for the ETA receptor were 0.07, 0.38, 0.80, 3.67 and 33.6 nM, resp. A similar hierarchy was revealed by the functional assays. Our results suggest that
the rank order of potency of the antagonists is A-127722 ≥ PD-156707 ≥ FR139317 > Ro-47-0203 > L-749329.
IT 162412-70-6, PD-156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(endothelin receptor antagonists: serum albumin effect on potency and comparison of pharmacol. characteristics)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA

L4 ANSWER 94 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)



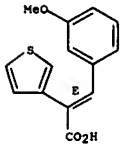
● Na

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:284248 CAPLUS
DOCUMENT NUMBER: 126:264101
TITLE: Preparation of acryloylguanidine derivatives as Na+/H+ exchanger inhibitors
INVENTOR(S): Kikuchi, Kazumi; Toyoshima, Akira; Okazaki, Toshio; Takanashi, Masahiro; Yanagisawa, Isao
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

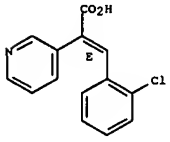
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9711055	A1	19970327	WO 1996-JP2696	19960919
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ZA 9607800	A	19970403	ZA 1996-7800	19960916
CA 2232497	A1	19970327	CA 1996-2232497	19960919
AU 9670007	A	19970409	AU 1996-70007	19960919
AU 702092	B2	19990211		
EP 861831	A1	19980902	EP 1996-931252	19960919
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1196721	A	19981021	CN 1996-196999	19960919
BR 9610530	A	19990706	BR 1996-10530	19960919
HU 9901336	A2	19990830	HU 1999-1336	19960919
HU 9901336	A3	20000228		
NO 9801241	A	19980520	NO 1998-1241	19980319
PRIORITY APPLN. INFO.:			JP 1995-241716 A	19950920
			WO 1996-JP2696 W	19960919

OTHER SOURCE(S): MARPAT 126:264101
AB The title compds. BCR1:CACON:C(NH2)2 [I; A = (un)substituted fused benzene ring, 5-6 numbered heterocyclyl; B = (un)substituted aryl; R1 = H, halo, optionally halogenated lower alkyl] are prepared I, possessing Na+/H+ exchanger inhibitory activity, are useful as a preventive, remedy or diagnostic drug for various diseases in which the Na+/H+ exchanger participates, for example, hypertension, arrhythmia, angina pectoris, arteriosclerosis, and complications of diabetes (no data). Thus, acryl acid derivs. BCH:CACOX [II; B = 3-MeOC6H4, A = thienyl, X = OH) was reacted with N:C(NH2)2 in the presence of 1,1'-carbonyldiimidazole in DMF to give the title compound II [A, B = same as above, X = N:C(NH2)2].
IT 141694-17-9P 188815-46-5P 188815-47-6P
188815-49-8P 188815-53-4P 188815-54-5P



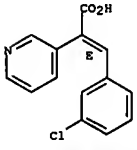
RN 188815-49-8 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-chlorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-53-4 CAPLUS
CN 3-Pyridineacetic acid, α-[(3-chlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

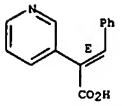


RN 188815-54-5 CAPLUS
CN 3-Pyridineacetic acid, α-[(4-chlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

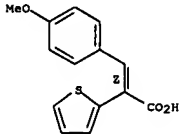
188815-55-6P 188815-56-7P 188815-57-8P
188815-58-9P 188815-60-3P 188815-61-4P
188815-62-5P 188815-63-6P 188815-64-7P
188815-65-8P 188815-66-9P 188815-67-0P
188815-68-1P 188815-69-2P 188815-70-5P
188815-71-6P 188815-74-9P 188815-75-0P
188815-76-1P 188815-77-2P 188815-78-3P
188815-79-4P 188815-80-7P 188815-82-9P
188815-83-0P 188815-84-1P 188815-85-2P
188815-86-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of acryloylguanidine derivs. as Na+/H+ exchanger inhibitors)
RN 141694-17-9 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



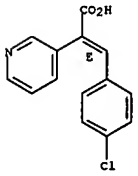
RN 188815-46-5 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-methoxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



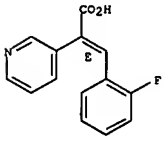
RN 188815-47-6 CAPLUS
CN 3-Thiopheneacetic acid, α-[(3-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



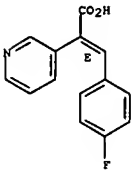
RN 188815-55-6 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-fluorophenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-56-7 CAPLUS
CN 3-Pyridineacetic acid, α-[(4-fluorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

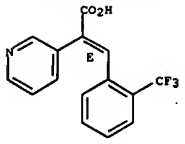
Double bond geometry as shown.



RN 188815-57-8 CAPLUS
CN 3-Pyridineacetic acid, α-[[2-(trifluoromethyl)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

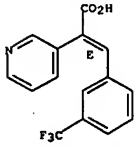
Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



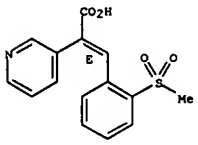
RN 188815-58-9 CAPLUS
CN 3-Pyridineacetic acid, α-[[3-(trifluoromethyl)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-60-3 CAPLUS
CN 3-Pyridineacetic acid, α-[[2-(methylsulfonyl)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

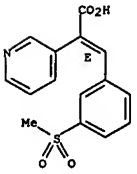
Double bond geometry as shown.



RN 188815-61-4 CAPLUS
CN 3-Pyridineacetic acid, α-[[3-(methylsulfonyl)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

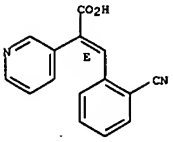
Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



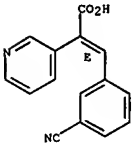
RN 188815-62-5 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-cyanophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



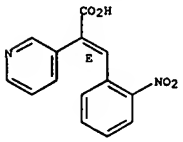
RN 188815-63-6 CAPLUS
CN 3-Pyridineacetic acid, α-[(3-cyanophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



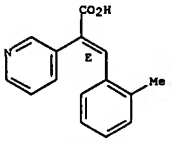
RN 188815-64-7 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-nitrophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



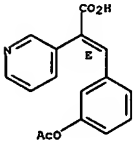
RN 188815-65-8 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-66-9 CAPLUS
CN 3-Pyridineacetic acid, α-[[3-(acetyloxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

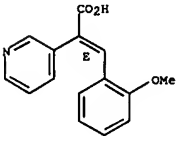
Double bond geometry as shown.



RN 188815-67-0 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

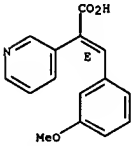
Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



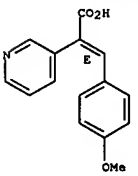
RN 188815-68-1 CAPLUS
CN 3-Pyridineacetic acid, α-[(3-methoxyphenyl)methylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-69-2 CAPLUS
CN 3-Pyridineacetic acid, α-[(4-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

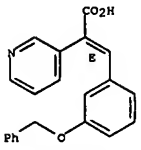
Double bond geometry as shown.



RN 188815-70-5 CAPLUS
CN 3-Pyridineacetic acid, α-[[3-(phenylmethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

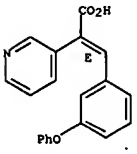
Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



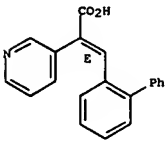
RN 188815-71-6 CAPLUS
CN 3-Pyridineacetic acid, α-[(3-phenoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-74-9 CAPLUS
CN 3-Pyridineacetic acid, α-([1,1'-biphenyl]-2-ylmethylene)-, (E)- (9CI) (CA INDEX NAME)

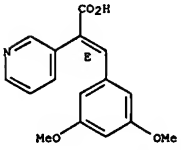
Double bond geometry as shown.



RN 188815-75-0 CAPLUS
CN 3-Pyridineacetic acid, α-([1,1'-biphenyl]-3-ylmethylene)-, (E)- (9CI) (CA INDEX NAME)

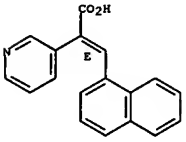
Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



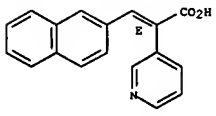
RN 188815-79-4 CAPLUS
CN 3-Pyridineacetic acid, α-(1-naphthalenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-80-7 CAPLUS
CN 3-Pyridineacetic acid, α-(2-naphthalenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



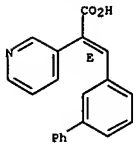
RN 188815-82-9 CAPLUS
CN 3-Pyridineacetic acid, α-[[3-[3-(1-piperidinyl)propoxy]phenyl]methylene]-, (E)-, monoformate (9CI) (CA INDEX NAME)

CM 1

CRN 188815-81-8
CMF C22 H26 N2 O3

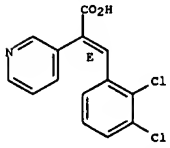
Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



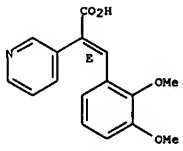
RN 188815-76-1 CAPLUS
CN 3-Pyridineacetic acid, α-[(2,3-dichlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 188815-77-2 CAPLUS
CN 3-Pyridineacetic acid, α-[(2,3-dimethoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

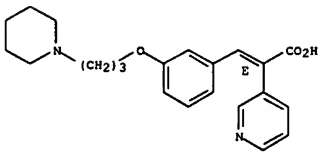
Double bond geometry as shown.



RN 188815-78-3 CAPLUS
CN 3-Pyridineacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



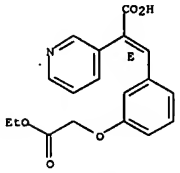
CM 2

CRN 64-18-6
CMF C H2 O2

O=CH-OH

RN 188815-83-0 CAPLUS
CN 3-Pyridineacetic acid, α-[[3-(2-ethoxy-2-oxoethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

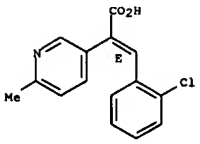
Double bond geometry as shown.



RN 188815-84-1 CAPLUS
CN 3-Pyridineacetic acid, α-[(2-chlorophenyl)methylene]-6-methyl-, (E)- (9CI) (CA INDEX NAME)

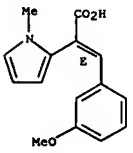
Double bond geometry as shown.

L4 ANSWER 95 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



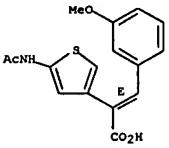
RN 188815-85-2 CAPLUS
CN 1H-Pyrrole-2-acetic acid, α-[(3-methoxyphenyl)methylene]-1-methyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

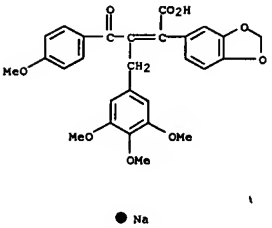


RN 188815-86-3 CAPLUS
CN 3-Thiopheneacetic acid, 5-(acetylamino)-α-[(3-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 96 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

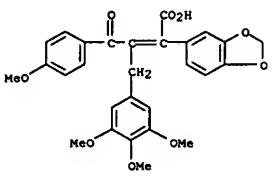


REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 96 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:282253 CAPLUS
DOCUMENT NUMBER: 126:338577
TITLE: Affinity and selectivity of PD156707, a novel nonpeptide endothelin antagonist, for human ETA and ETB receptors
AUTHOR(S): Maguire, Janet J.; Kuc, Rhoda E.; Davenport, Anthony P.
CORPORATE SOURCE: Clinical Pharmacology Unit, University of Cambridge, Addenbrooke's Hospital, Cambridge, CB2 2QQ, UK
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1997), 280(2), 1102-1108
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have determined the affinity and selectivity of a new nonpeptide antagonist PD156707 (sodium 2-benzo(1,3)dioxol-5-yl-4-(4-methoxy-phenyl)-4-oxo-3-(3,4,5-trimethoxybenzyl)-but-2-enolate) for human endothelin (ET)A and ETB receptors. In human coronary artery and saphenous vein the affinity of the ETA receptor for PD156707 was 0.15 ± 0.06 nM and 0.5 ± 0.13 nM, resp. Competition expts. in human left ventricle and kidney revealed that PD156707 had 1,000- to 15,000-fold selectivity for the ETA receptor over the ETB receptor. This selectivity was confirmed autoradiog. In human coronary artery, mammary artery and saphenous vein PD156707 (3-300 nM) potently antagonized the vasoconstrictor responses to ET-1. The pA2 values estimated from the Gaddum-Schild equation were 8.07 ± 0.09, 8.45 ± 0.11 and 8.70 ± 0.13, resp. The concentration-response curves to ET-1 were shifted to the right in parallel fashion, without reduction of the maximum response. However, the regression lines fitted to the resulting Schild data deviated significantly from one. PD156707 appeared to be a more effective antagonist at lower concns. than at the higher ones. It is possible that PD156707, a sodium salt, was reverting to a less soluble form which results in underestimation of its potency. These data show that PD156707 is a potent and selective antagonist at human ETA receptors and will be useful in clarifying the role of the endothelin peptides in human cardiovascular disease.
IT 162412-70-6, PD156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(endothelin antagonist PD156707 affinity and selectivity for ETA and ETB receptors)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 97 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:272682 CAPLUS
DOCUMENT NUMBER: 126:315774
TITLE: Concomitant endothelin receptor subtype-A blockade during the progression of pacing-induced congestive heart failure in rabbits. Beneficial effects on left ventricular and myocyte function
AUTHOR(S): Spinale, Francis G.; Walker, Jennifer D.; Mukherjee, Rupak; Iannini, Julie P.; Keever, Anthony T.; Gallagher, Kim P.
CORPORATE SOURCE: Division of Cardiothoracic Surgery, Medical University of South Carolina, Charleston, SC, 29425, USA
SOURCE: Circulation (1997), 95(7), 1918-1929
CODEN: CIRCAZ; ISSN: 0009-7322
PUBLISHER: American Heart Association
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Plasma levels of endothelin-1 (ET-1) are increased in patients and animals with severe congestive heart failure (CHF). It remains unknown, however, whether ET-1 plays a direct and contributory role in the progression of CHF. Accordingly, the present project tested the hypothesis that chronic blockade of the ETA receptor would have direct and beneficial effects on left ventricular (LV) and myocyte function in a model of CHF. Global LV and isolated myocyte function were examined in rabbits in the following groups (12 per group): chronic rapid ventricular pacing (RVP; 400 bpm, 3 wk), RVP and concomitant administration of the selective ETA receptor antagonist (PD 156707 24 mg/d), and sham controls. LV fractional shortening decreased after RVP (17±5 vs. 42±3%) and end-diastolic dimension increased (2.36±0.44 vs. 1.24±0.18 cm) compared with controls (P<.05). With RVP plus ETA blockade, LV fractional shortening was increased (33±6%) and end-diastolic dimension decreased (2.02±0.30 cm) compared with RVP-only values (P<.05). Plasma norepinephrine and endothelin increased twofold in the RVP group. In the RVP plus ETA blockade group, plasma endothelin increased threefold compared with RVP values. Isolated myocyte shortening velocity declined after RVP (42±13 vs. 72±10 μm/s, P<.05) compared with controls but was normalized with RVP plus ETA blockade (77±16 μm/s). Myocyte inotropic response to extracellular Ca2+, β-receptor stimulation, and ET-1 was reduced in the RVP group and returned to control levels with RVP and concomitant ETA receptor blockade. The results from this study suggest that chronically elevated ET-1 levels and subsequent activation of the ETA receptor play a direct and contributory role in the progression of the CHF process. Thus, specific ETA receptor blockade may provide a new and useful therapeutic modality in the setting of CHF.
IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin receptor subtype-A blockade during progression of pacing-induced congestive heart failure)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX

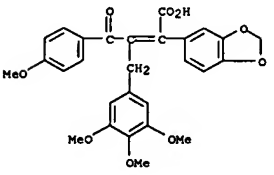
L4 ANSWER 97 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)



● Na

L4 ANSWER 98 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:215718 CAPLUS
DOCUMENT NUMBER: 126:220307
TITLE: Structure-Activity Relationships in a Series of Orally
Active γ-Hydroxy Butenolide Endothelin Antagonists
AUTHOR(S): Patt, William C.; Edmunds, Jeremy J.; Repine, Joseph T.; Berryman, Kent A.; Reisdorph, Billy R.; Lee, Chet;
Plummer, Mark S.; Shahripour, Aurash; Haleen, Stephen J.; Keiser, Joan A.; Flynn, Mike A.; Welch, Kathleen M.; Reynolds, Elwood E.; Rubin, Ron; Tobias, Brian; Hallak, Hussein; Doherty, Annette M.
CORPORATE SOURCE: Department of Medicinal Chemistry Park-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (1997), 40(7), 1063-1074
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The design of potent and selective non-peptide antagonists of endothelin-1
(ET-1) and its related isopeptides are important tools defining the role of ET in human diseases. In this report we will describe the detailed structure-activity relationship (SAR) studies that led to the discovery of
a potent series of butenolide ETA selective antagonists. Starting from a micromolar screening hit, PD012527, use of Topliss decision tree anal. led
to the discovery of the nanomolar ETA selective antagonist PD155080. Further structural modifications around the butenolide ring led directly to the subnanomolar ETA selective antagonist PD156707, IC50's = 0.3 (ETA) and 780 nM (ETB). This series of compds. exhibited functional activity exemplified by PD156707. This derivative inhibited the ETA receptor mediated
release of arachidonic acid from rabbit renal artery vascular smooth muscle cells with an IC50 = 1.1 nM and also inhibited the ET-1 induced contraction of rabbit femoral artery rings (ETA mediated) with a pA2 = 7.6. PD156707 also displayed in vivo functional activity inhibiting the hemodynamic responses due to exogenous administration of ET-1 in rats in a
dose dependent fashion. Evidence for the pH dependence of the open and closed tautomerization forms of PD156707 was demonstrated by an NMR study.
X-ray crystallog. anal. of the closed butenolide form of PD156707 shows the benzylic group located on the same side of the butenolide ring as the γ-hydroxyl and the remaining two Ph groups on the butenolide ring essentially orthogonal to the butenolide ring. Pharmacokinetic parameters
for PD156707 in dogs are also presented.
IT 162412-70-6P, PD 156707
RL: BAC (Biological activity or effector, except adverse); BPR (Biological

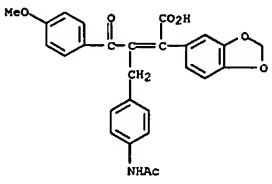
L4 ANSWER 98 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. of and endothelin-antagonistic structure-activity relationship of γ-hydroxy butenolides)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX
NAME)



● Na

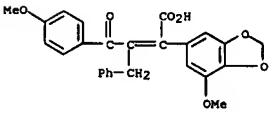
IT 169805-68-9P 169805-70-3P 169805-71-4P
169805-73-6P 169805-89-4P 188395-16-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of and endothelin-antagonistic structure-activity relationship
of γ-hydroxy butenolides)
RN 169805-68-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[4-(acetylamino)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, monopotassium salt (9CI) (CA INDEX
NAME)

L4 ANSWER 98 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● K

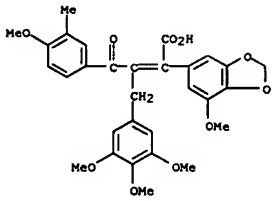
RN 169805-70-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

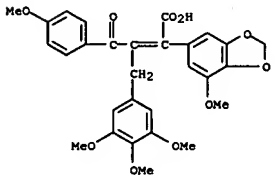
RN 169805-71-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium
salt (9CI) (CA INDEX NAME)

L4 ANSWER 98 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 169805-73-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

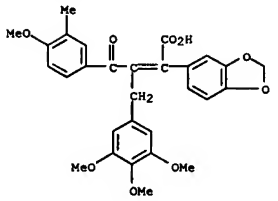


● Na

RN 169805-89-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 98 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued).

L4 ANSWER 98 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

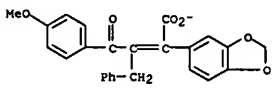


● Na

RN 188395-16-6 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 188395-15-5
CMF C25 H19 O6



CM 2

CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N-CH_2-CH_2-OH$

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 99 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

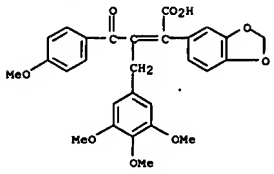
ACCESSION NUMBER: 1997:196059 CAPLUS
DOCUMENT NUMBER: 126:272067
TITLE: Effects of endothelin ETA receptor antagonism with PD 156707 on hemodynamics and renal vascular resistance in rabbits
AUTHOR(S): Ignasiak, Diane P.; McClanahan, Thomas B.; Saganek, Lori J.; Potoczak, Ronald E.; Hallak, Hussein; Gallaher, Kim P.
CORPORATE SOURCE: Parke-Davis Pharmaceutical Res., Div. Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: European Journal of Pharmacology (1997), 321(3), 295-300
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The objective of this study was to determine the in vivo effectiveness of selective endothelin ETA receptor antagonist PD 156707 [sodium 2-benzo[1,3]dioxol-5-yl-4-(4-methoxyphenyl)-4-oxo-3-(3,4,5-trimethoxybenzyl)but-2-enoate]. Effectiveness was defined by the ability of the compound to block increases in renal vascular resistance and mean arterial blood pressure induced by an i.v. bolus of 0.3 nmol/kg of human endothelin-1 in pentobarbital anesthetized rabbit. Different groups of rabbit received hour long i.v. infusion of PD 156707 at dose of 0.003, 0.01, 0.03 or 0.3 mg/kg/h. During baseline conditions, mean arterial blood pressure, heart rate, renal blood flow, and renal vascular resistance were similar among the groups. The i.v. bolus of endothelin-1-significantly decrease mean arterial blood pressure (82±3 mmHg to 65±3 mmHg) and increased renal vascular resistance (2.8±0.3 mmHg/mL/min to 9.2±1.1 mmHg/mL/min) in untreated control animals. At doses of 0.3 and 0.03 mg/kg/h, PD 156707 virtually abolished endothelin-1 increases in renal vascular resistance, but did not affect the endothelin-1 induced decrease in mean arterial blood pressure. At 0.01 and 0.003 mg/kg/h, PD 156707 also inhibited endothelin 1 induced increase in renal vascular resistance but the effects were less striking, leading to the conclusion that the min. effective i.v. dose of the compound in rabbits is in the range of 0.01-0.03 mg/kg/h. The results of this study demonstrate that PD 156707 is an extremely potent and highly selective endothelin ETA receptor antagonist. In addition, this study demonstrates the utility of renal vascular resistance as an in vivo bioassay for evaluating selective vascular effects of endothelin receptor antagonist in this species.

IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effects of endothelin ETA receptor antagonism with PD 156707 on hemodynamics and renal vascular resistance in rabbits)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

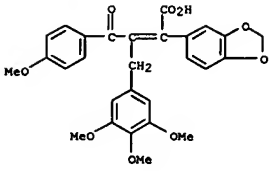
L4 ANSWER 99 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

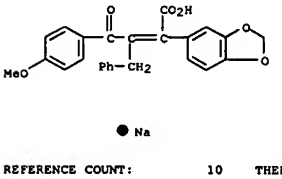
L4 ANSWER 100 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:119484 CAPLUS
DOCUMENT NUMBER: 126:211986
TITLE: γ-Carbamate butenolide analogs as potent ETA selective endothelin receptor antagonists and prodrugs
AUTHOR(S): Patt, William C.; Reisdorph, Billy R.; Repine, Joseph T.; Doherty, Annette M.; Haleen, Stephen J.; Walker, Donnelle M.; Welch, Kathleen M.; Flynn, Michael A.; Hallak, Hussein; Reyner, Eric L.; Stewart, Barbra H.
CORPORATE SOURCE: Dep. Medicinal Chemistry, Parke-Davis Pharmaceutical Res., Warner-Lambert Co., Ann Arbor, MI, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(3), 297-302
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Continued SAR around an ETA selective series of butenolide antagonists, for example PD156707 (1) has yielded a new series of subnanomolar ETA selective antagonists. Depending upon solution pH, 1 exists as the ring closed butenolide form or as the tautomeric open chain keto-acid salt. Reaction of butenolide γ-hydroxyl with isocyanates yields carbamates with essentially identical EtA binding affinity and with improved ETA selectivity. As carbamates these derivs. may undergo facile hydrolysis, reverting back to their parent butenolides, and therefore may be useful as prodrugs of 1. Stability studies of PD163140 (7) indicate that the compound is stable in the binding assay conditions and hence has intrinsic activity. In addition 7 is readily hydrolyzed by rat intestinal perfusate to yield the parent compound 1.
IT 162412-70-6P, PD156707 162412-71-7P, PD155080
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(γ-carbamate butenolide analogs as potent ETA selective endothelin receptor antagonists and prodrugs)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 100 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

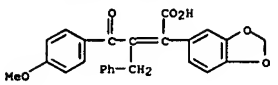


● Na

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 101 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:43874 CAPLUS
DOCUMENT NUMBER: 126:152570
TITLE: Effects of Ro 47-0203 and PD155080 on the plasma kinetics, receptor binding and vascular effects of endothelin in the pig
AUTHOR(S): Hemsen, Anette; Modin, Agnes; Wanecek, Michael; Malmstroem, Rickard E.; Weitzberg, Eddie
CORPORATE SOURCE: Division of Pharmacology, Department of Physiology and Pharmacology, Karolinska Institutet, Stockholm, S-17177, Swed.
SOURCE: European Journal of Pharmacology (1996), 318(2/3), 369-376
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effects of the mixed endothelin ETA/endothelin ETB receptor antagonist Ro 47-0203 (bosentan) and the selective endothelin ETA receptor antagonist PD155080 on plasma half-life and regional extraction of exogenous endothelin-1 as well as on the regional vascular effects of endothelin-1 were investigated in the pig in vivo. Bosentan but not PD155080 (5 mg/kg, i.v. bolus, both drugs) increased the arterial plasma levels of endothelin-1-like immunoreactivity. Neither of the drugs affected the plasma half-life of infused endothelin-1. In the spleen, both the extraction and vascular effects of exogenous endothelin-1 were attenuated by both bosentan and PD155080 whereas renal extraction and vascular effects in the kidney were unaffected by both drugs. In the lung, only bosentan decreased pulmonary extraction of endothelin-1. In conclusion, the bosentan-induced increase of circulating endothelin-1 seems to be related to blockade of endothelin-1 binding to endothelin ETB receptors. Blockade of these receptors does not influence the overall elimination of endothelin-1, however.
IT 162412-71-7, PD155080
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effects of Ro 47-0203 and PD155080 on plasma kinetics, receptor binding and vascular effects of endothelin)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 101 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

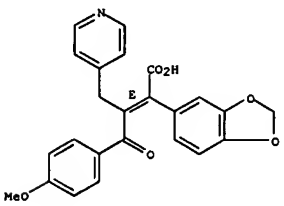
L4 ANSWER 102 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:612741 CAPLUS
DOCUMENT NUMBER: 125:247817
TITLE: Preparation of 4-(phenyl, thienyl, or dihydrobenzofuranyl)-3-(heterocyclylmethyl)-4-oxo-2-butenoic acid derivatives as endothelin antagonists
INVENTOR(S): Ishikawa, Kiyofumi; Nagase, Toshio; Ihara, Masaki; Nishikibe, Masaru
PATENT ASSIGNEE(S): Japan
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9623773	A1	19960808	WO 1996-JP195	19960201
W: AU, CA, CN, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9645478	A	19960821	AU 1996-45478	19960201
PRIORITY APPLN. INFO.:			JP 1995-39357	A 19950203
			WO 1996-JP195	W 19960201

OTHER SOURCE(S): MARPAT 125:247817
AB The title compds. represented by formula Ar1COC(CH2Ar2):CAr3CO2H (Ar1, Ar3 = each Ph, thienyl or dihydrobenzofuranyl optionally having 1 to 4 substituents; Ar2 = pyridyl, imidazolyl, thiazolyl, pyrimidinyl, pyridazinyl or pyrazinyl wherein an arbitrary hydrogen atom on its heterocycle may be substituted by C1-6 alkyl or C1-6 alkylamino) or pharmaceutically acceptable salts or esters thereof are prepared Because of having a potent antagonism on 3 endothelins (endothelin-1, -2, and -3) which are endogenous physiol. active peptides, the compds. are useful as drugs antagonistic to blood vessel and tracheal muscle contraction in which endothelin participates and, in turn, as remedies for human hypertension, pulmonary hypertension, Raynaud's disease, bronchial asthma, arteriosclerosis, acute renal insufficiency, cardiac insufficiency, myocardial infarction, angina pectoris, cerebral infarction, cerebrovascular spasm, gastric ulcer, and diabetes. They are also useful as remedies for reconstriction, prostatic hypertrophy, endotoxin shock, multiple organ failure or disseminated intravascular coagulation caused by endotoxins, cyclosporin-induced renal disorder, and hypertension. Thus, to a solution of 100 mg Me 4-(4-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)-4-oxobutanoate (preparation given) and 28 μL 4-pyridinecarboxaldehyde in MeOH was added a MeOH solution of NaOMe and the resulting mixture was stirred at 60° for 2.5 h, treated with another portion of the NaOMe solution, and stirred for 30 min to give, after workup and silica gel chromatog., 68.0

L4 ANSWER 102 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
mg 5-hydroxy-5-(4-methoxyphenyl)-3-(3,4-methylenedioxyphenyl)-4-(4-pyridylmethyl)-2(5H)-furanone (I) and 34.8 mg (E)-4-(4-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)-4-oxo-3-(4-pyridylmethyl)-2-butenoic acid (II).
To a soln. of 27 mg I in 0.5 mL MeOH and 0.3 mL 1,4-dioxane was added 60 μL 1 M aq. NaOH and the resulting mixt. was stirred at room temp. for 20 min to give II.Na. II.Na at 1.1. μM in vitro inhibited 99.5% binding of 125I-endothelin-1 to the endothelin receptor of membranes of human neuroblastoma-derived SK-N-MC cells.
IT 181936-39-0P 181936-41-4P 181936-48-1P
181936-52-7P 181936-58-3P 181936-63-0P
181936-67-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (Ph, thienyl, or dihydrobenzofuranyl)(heterocyclylmethyl)oxobutenoic acid derivs. as endothelin antagonists for disease therapy)
RN 181936-39-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(4-pyridinylmethyl)ethylidene]-, (E)- (9CI) (CA INDEX NAME)

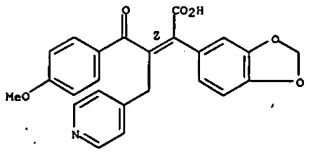
Double bond geometry as shown.



RN 181936-41-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(4-pyridinylmethyl)ethylidene]-, sodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

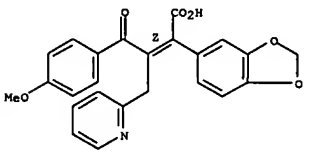
L4 ANSWER 102 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 181936-48-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(2-pyridinylmethyl)ethylidene]-, sodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

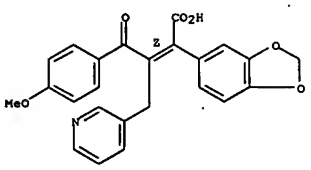


● Na

RN 181936-52-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(3-pyridinylmethyl)ethylidene]-, sodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

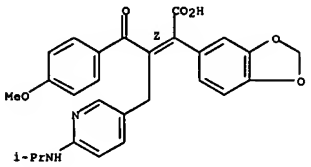
L4 ANSWER 102 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 181936-58-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[[6-[(1-methylethyl)amino]-3-pyridinyl]methyl]-2-oxoethylidene]-, monosodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

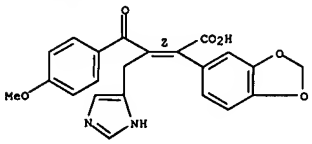


● Na

RN 181936-63-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-(1H-imidazol-4-ylmethyl)-2-(4-methoxyphenyl)-2-oxoethylidene]-, monosodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

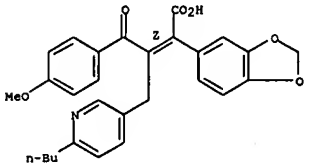
L4 ANSWER 102 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 181936-67-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(6-butyl-3-pyridinyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● Na

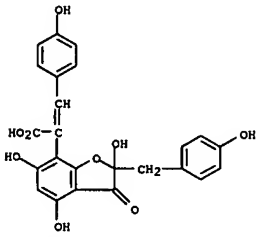
L4 ANSWER 103 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:599446 CAPLUS
DOCUMENT NUMBER: 125:270472
TITLE: Benzofuranoids with carbon frameworks reminiscent of products of benzylic acid rearrangement
AUTHOR(S): Bekker, Riaan; Smit, Rachel S.; Brandt, E. Vincent; Ferreira, Daneel
CORPORATE SOURCE: Dep. Chem., Univ. Orange Free State, Bloemfontein, 9300, S. Afr.
SOURCE: Phytochemistry (1996), 43(3), 673-679
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

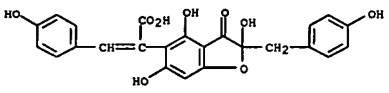
AB The heartwood of Berchemia zeyheri yielded 4,6-dihydroxy-3-(4-hydroxybenzyl)-3-methylbenzo[b]-furan-2(3H)-one and the 5- and 7-[2-(4-coumaroyl)]maesopsins, benzofuranoid-type flavonoids with mol. backbones reminiscent of products of benzylic acid rearrangement.

IT 182057-54-1 182057-61-0
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(benzofuranoids from Berchemia zeyheri)

RN 182057-54-1 CAPLUS
CN 7-Benzofuranacetic acid, 2,3-dihydro-2,4,6-trihydroxy-2-[(4-hydroxyphenyl)methyl]-α-[(4-hydroxyphenyl)methylene]-3-oxo- (9CI) (CA INDEX NAME)



RN 182057-61-0 CAPLUS
CN 5-Benzofuranacetic acid, 2,3-dihydro-2,4,6-trihydroxy-2-[(4-hydroxyphenyl)methyl]-α-[(4-hydroxyphenyl)methylene]-3-oxo- (9CI) (CA INDEX NAME)



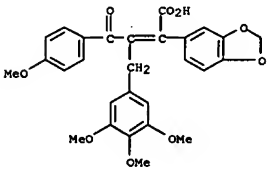
L4 ANSWER 103 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 104 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:586655 CAPLUS
DOCUMENT NUMBER: 125:238442
TITLE: Endothelin receptor antagonist increases cerebral perfusion and reduces ischemic damage in feline focal cerebral ischemia
AUTHOR(S): Patel, Toshal R.; Galbraith, Samuel; Graham, David I.; Hallak, Hussein; Doherty, Annette M.; McCulloch, James
CORPORATE SOURCE: Wellcome Surgical Institute, University Glasgow, Glasgow, G61 1QH, UK
SOURCE: Journal of Cerebral Blood Flow and Metabolism (1996), 16(5), 950-958
CODEN: JCBMDN; ISSN: 0271-678X
PUBLISHER: Lippincott-Raven
DOCUMENT TYPE: Journal
LANGUAGE: English

AB These investigations characterized the cerebrovascular effects of an endothelin ETA-receptor antagonist PD156707 in normal and ischemic cat brain. A dose of PD156707 that inhibited the effects of exogenous endothelin-1 was established in nonischemic cerebral resistance arterioles. Perivascular microapplication of the endothelin-receptor antagonist PD156707 (0.03-3 μM) had a minimal effect on nonischemic pial resistance arterioles. The perivascular coapplication of PD156707 and ET-1 (10 nM) effected a dose-dependent attenuation of the ET-1 vasoconstrictive response (IC50 = 0.1 μM). I.v. administration of PD156707 (3 μmol/kg bolus + 5 μmol/kg/h infusion) attenuated the vasoconstriction elicited by perivascular ET-1 (10 nM) in normal pial arterioles (ET-1 vasoconstriction: -37 ± 13% from preinjection baseline; after i.v. PD156707: 6 ± 10% from preinjection baseline). In the focal ischemia studies, cerebral perfusion was measured in the suprasylvian and ectosylvian gyri (by laser Doppler flowmetry). Occlusion of the middle cerebral artery reduced cerebral perfusion in the suprasylvian and ectosylvian gyri by .apprx.50%. I.v. administration of PD156707 (3 μmol/kg bolus + 5 μmol/kg/h infusion), initiated 30 min after middle cerebral artery occlusion, effected a progressive increase in cerebral perfusion up to preocclusion baseline levels, whereas cerebral perfusion in vehicle-treated animals did not vary from its postocclusion level. In these animals, the i.v. administration of PD156707 reduced the hemispheric volume of ischemic damage by 45% (vehicle: 2,376 ± 1,107 mm3; PD156707: 1,307 ± 548 mm3; p < 0.05). Our investigations indicate that endothelin receptor antagonism may be a new therapeutic strategy for the amelioration of focal ischemic damage.

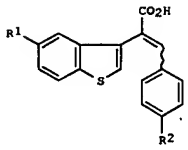
IT 162412-70-6, PD156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(endothelin receptor antagonist PD156707 increases cerebral perfusion and reduces ischemic damage in focal cerebral ischemia)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

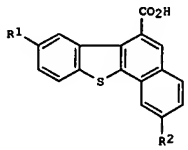


● Na

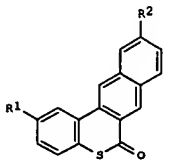
L4 ANSWER 105 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:582779 CAPLUS
DOCUMENT NUMBER: 125:300701
TITLE: Photocyclization of 2-([1]benzothien-3-yl)-3-phenylpropenoic acids
AUTHOR(S): Tominaga, Yoshinori; Castle, Lyle W.; Castle, Raymond N.
CORPORATE SOURCE: Fac. Pharmacetuical Sci., Nagasaki Univ., Nagasaki, 852, Japan
SOURCE: Journal of Heterocyclic Chemistry (1996), 33(4), 1319-1321
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:300701
GI



I



II

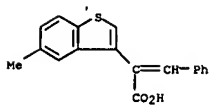


III

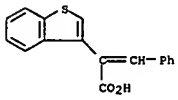
AB Photocyclization of the substituted 2-([1]benzothien-3-yl)-3-phenylpropenoic acids I (R1 = R2 = H; R1 = Me, R2 = H, OMe) in the presence of iodine and air in a benzene-cyclohexane mixture afforded a separable mixture of three compds., benzo[b]naphtho[2,1-d]thiophene-6-carboxylic acids II, 6H-benzo[b]naphtho[2,3-d]thiopyran-6-ones III, and 10-methoxy-2-methyl-6H-benzo[b]naphtho[2,3-d]pyran-6-one.

IT 83821-47-0P 183018-47-5P 183018-48-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photocyclization of benzothienylphenylpropenoic acids)

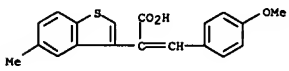
RN 83821-47-0 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, 5-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 183018-47-5 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



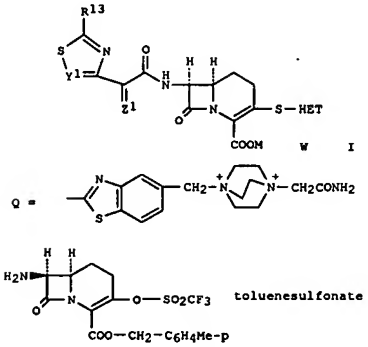
RN 183018-48-6 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, α-[(4-methoxyphenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 106 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:527732 CAPLUS
DOCUMENT NUMBER: 125:195285
TITLE: Preparation of 3-(heteroarylthio)-1-carba-1-dethiacephalosporins as antibacterials
INVENTOR(S): Cama, Lovji D.; Hammond, Milton L.; Sasor, Mary F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 59 pp., Division of U.S. Ser. 391,857.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5538964	A	19960723	US 1995-463489	19950605
US 5565445	A	19961015	US 1995-391857	19950222
PRIORITY APPLN. INFO.:			US 1995-391857	A3 19950222

OTHER SOURCE(S): MARPAT 125:195285
GI

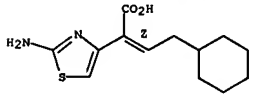


AB 1-Carba-1-dethiacephalosporin compds. [I; Y1 = CH or N; M = hydrogen, a neg. charge, a bio-labile ester forming group or a carboxyl protecting group; R13 = (un)substituted imino; W is present or absent, and when present, it represents a neg. charged counter-ion; Z1 = (alkyl)methylene, cycloalkylmethylene, etc.; HET = a heterocyclic group with from one to three pos. charged atoms], useful as antibacterials (no data), are prepd. E.g., I [Y1 = CH, R13 = NH2, Z1 = (Z)-N-CH2-CH2-F, COOM = COO-, HET = Q, W = Cl-] was prepd. in many steps via II. The compds. are useful against MRSA/MRCNS. Methods of use and preferred dosages are given.

IT 147699-51-2 181025-71-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 3-(heteroarylthio)carbadethiacephalosporins as antibacterials)

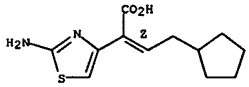
RN 147699-51-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(2-cyclohexylethylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 181025-71-8 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(2-cyclopentylethylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



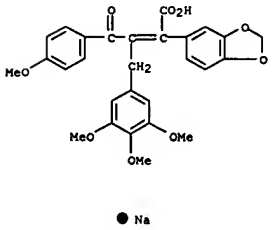
L4 ANSWER 107 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:435289 CAPLUS
DOCUMENT NUMBER: 125:132130
TITLE: EndothelinA receptor antagonism by PD 156707 does not reduce infarct size after coronary artery occlusion/reperfusion in pigs
AUTHOR(S): Mertz, Thomas E.; McClanahan, Thomas B.; Flynn, Michael A.; Juneau, Paul; Reynolds, Elwood E.; Hallak, Hussein; Bradford, Laura; Gallagher, Kim P.
CORPORATE SOURCE: Div. Warner-Lambert Co., Parke-Davis Pharm. Res., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1996), 278(1), 42-49
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Episodes of myocardial ischemia are associated with increases in cardiac venous plasma endothelin (ET) concns., suggesting that ET may play a role in the development of myocardial infarction. The purpose of this study was to determine if selective blockade of ETA receptors by PD 156707 reduces infarct size caused by coronary artery occlusion and reperfusion in pentobarbital-anesthetized micropigs. A PD 156707 dose which selectively blocks the ETA-mediated vasopressor response, but not the ETB-mediated vasodepressor response to i.v. ET-1 challenges (0.3 nmol/kg), was established in dose ranging studies in anesthetized micropigs. In myocardial infarction studies, micropigs received either saline vehicle (n = 7) or PD 156707 (n = 8) at a loading dose of 10 mg/kg/1 h, followed by a maintenance dose of 7 mg/kg/h. Coinciding with the start of the maintenance dose, the left anterior descending coronary artery was occluded for 1 h followed by 3 h of reperfusion. PD 156707 caused a significant (29 mm Hg) decrease in arterial blood pressure before occlusion. PD 156707 had no effect on infarct size (61.1 ± 5.6% of the region at risk in the PD 156707 treatment group vs. 70.1 ± 3.9% in the control group). These results suggest that ETA receptor activation does not substantially contribute to coronary artery occlusion/reperfusion-induced myocardial infarction.

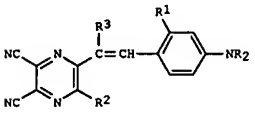
IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effect of endothelinA receptor antagonism by PD 156707 on infarct size after coronary artery occlusion/reperfusion)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 107 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 108 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:382181 CAPLUS
DOCUMENT NUMBER: 125:89144
TITLE: Syntheses and properties of new styryl dyes derived from 2,3-dicyano-5-methylpyrazines
AUTHOR(S): Jaung, Jae-yun; Matsuoka, Masaru; Fukunishi, Koushi
CORPORATE SOURCE: Dep. Chemistry, Kyoto Inst. Technol., Kyoto, 606, Japan
SOURCE: Dyes and Pigments (1996), 31(2), 141-153
CODEN: DYPIDX; ISSN: 0143-7208
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:89144
GI



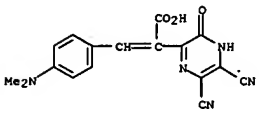
I

AB Reaction of 2,3-dicyano-5-methylpyrazine derivs. with aryl aldehydes gave new fluorescent styryl dyes (I; R = Me, Et; R1 = H, Me, OH; R2 = OH, OAc, Me, H; R3 = H, CO2H). These styryl dyes have extended π-conjugated systems and are strong intramol. charge-transfer chromophoric systems. The styryl dyes derived from 2,3-dicyano-6-hydroxy-5-methylpyrazine showed large solvatochromism, depending on the polarity of the solvent, due to tautomerism between the hydroxypyrazine and the pyridone forms. The fluorescence and solvatochromism properties of the dyes were also studied, and structure-property relationships in solution and in the solid state were evaluated on the basis of mol. stacking in the solid state.

IT 178920-57-5P
RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(syntheses and properties of styryl dyes derived from 2,3-dicyano-5-methylpyrazines)

RN 178920-57-5 CAPLUS
CN Pyrazineacetic acid, 5,6-dicyano-α-[[4-(dimethylamino)phenyl]methylene]-3,4-dihydro-3-oxo- (9CI) (CA INDEX NAME)

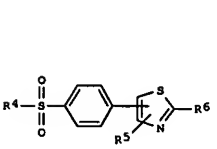
L4 ANSWER 108 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



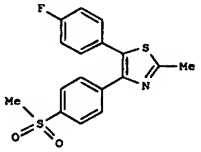
L4 ANSWER 109 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:353214 CAPLUS
DOCUMENT NUMBER: 125:33628
TITLE: Substituted thiazoles for the treatment of inflammation
INVENTOR(S): Talley, John J.; Carter, Jeffery S.; Collins, Paul W.; Kramer, Steven W.; Penning, Thomas D.; Rogier, Donald J., Jr.; Rogers, Roland S.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: PCT Int. Appl., 220 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9603392	A1	19960208	WO 1995-US9444	19950726
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2195847	A1	19960208	CA 1995-2195847	19950726
AU 9532010	A	19960222	AU 1995-32010	19950726
EP 772606	A1	19970514	EP 1995-928145	19950726
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 10504542	T	19980506	JP 1995-505961	19950726
EP 1125932	A2	20010822	EP 2001-112264	19950726
EP 1125932	A3	20010829		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
US 5668161	A	19970916	US 1996-679462	19960709
PRIORITY APPLN. INFO.:			US 1994-281288 A	19940727
			EP 1995-928145 A3	19950726
			WO 1995-US9444 W	19950726

OTHER SOURCE(S): MARPAT 125:33628
GI



I



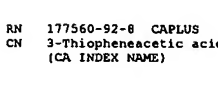
II

L4 ANSWER 109 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

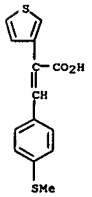
AB A class of substituted thiazolyl compds. is described, useful for treatment of inflammation and related disorders (arthritis, pain, and fever). Compds. of particular interest are I [R4 = alkyl and amino; R5 = (un)substituted aryl, cycloalkyl, cycloalkenyl, and heterocyclyl; R6 = halo, (un)substituted amino, (un)substituted alkoxy, NO2, OH, substituted carbonyl, acyl, alkenyl, alkynyl, (un)substituted alkyl, (un)substituted aryl or heterocyclyl] and their pharmaceutically acceptable salts. For example, Friedel-Crafts acylation of MeSPh with 4-FC6H4CH2COCl gave 48% 4-MeSC6H4COCH2C6H4F-4, which underwent a sequence of α-bromination (69%), cyclocondensation with thioacetamide (68%), and S-oxidation with m-ClC6H4C(O)OOH (57%), to give a preferred title compound, II. In the carrageenan-induced rat paw edema test, II gave 48% inhibition at 20 mg/kg orally. Examples include 65 addnl. syntheses, edema and analgesia assays in vivo, and selective inhibition of recombinant cyclooxygenase 2 in vitro.

IT 177560-88-2P 177560-92-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of substituted thiazoles as antiinflammatories)

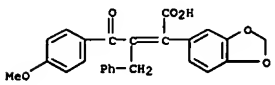
RN 177560-88-2 CAPLUS
CN 2-Thiopheneacetic acid, α-[[4-(methylthio)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 177560-92-8 CAPLUS
CN 3-Thiopheneacetic acid, α-[[4-(methylthio)phenyl]methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 110 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:275828 CAPLUS
DOCUMENT NUMBER: 124:331179
TITLE: Therapeutic potential of endothelin receptor antagonists in cerebrovascular disease
AUTHOR(S): Patel, Toshal R.
CORPORATE SOURCE: Wellcome Surgical Institute, University Glasgow, Glasgow, UK
SOURCE: CNS Drugs (1996), 5(4), 293-310
CODEN: CNDREF; ISSN: 1172-7047
PUBLISHER: Adis
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 178 refs. The actions of the endothelins (endothelin-1, endothelin-2 and endothelin-3) are mediated via endothelin-A (ETA) and endothelin-B (ETB) receptors, the former generally mediating vasoconstriction and the latter vasodilation. Peptide antagonists selective for either receptor subtype [e.g. BQ 123 (ETA) and BQ 788 (ETB)] and combined ETA/ETB receptor antagonists (e.g. PD 145065 and TAK 044) have been developed. More recently, small mol. non-peptide antagonists have also been synthesized. ETA receptor-selective agents include PD 155080 and BMS 182874, while Ro 46-2005 and bosentan are combined ETA/ETB receptor antagonists. The role of the endothelin family of vasoconstrictor peptides in the pathophysiol. of cerebrovascular disease has been speculated upon. Increases in plasma and CSF levels of endothelin-1 in delayed vasospasm following subarachnoid hemorrhage and acute ischemic stroke have implicated the endothelins in these cerebrovascular diseases. The development of non-peptide endothelin receptor.
IT 162412-71-7, PD 155080
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic potential of endothelin receptor antagonists in cerebrovascular disease)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

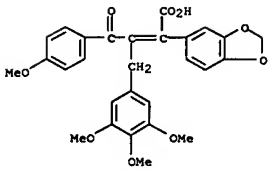


● Na

L4 ANSWER 110 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 111 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:269517 CAPLUS
DOCUMENT NUMBER: 124:308510
TITLE: Endothelins and endothelin receptor antagonists: binding to plasma proteins
AUTHOR(S): Wu-Wong, Jinshyun R.; Chiou, William J.; Hoffman, Daniel J.; Winn, Martin; von Geldern, Thomas W.; Opgenorth, Terry J.
CORPORATE SOURCE: Pharmaceutical Products Division, Abbott Laboratories, Abbott Park, IL, 60064, USA
SOURCE: Life Sciences (1996), 58(21), 1839-47
CODEN: LIFSAK; ISSN: 0024-3205
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Endothelins (ET) are 21-amino acid peptides that bind to membrane receptors to initiate a wide range of pathophysiol. effects. PD-156707, L-749329, Ro-47-0203, and A-127722 are potent non-peptide ET receptor antagonists developed recently. When tested in human and rat plasma, both ET-1 and -3 and the four aforementioned antagonists exhibited a high degree (>98%) of plasma protein binding. When ET-1 binding to the receptors was examined, 5% (volume/volume) of human plasma inhibited ET-1 binding to both ETA and ETB receptors by 80-90%. Similarly, 5% (w/v) of human serum albumin inhibited ET-1 binding by 82%, suggesting that the major protein component in plasma which interfered with ET-1 binding to the receptors was serum albumin. Competition studies show that, in the absence of human serum albumin, the IC50 values of PD-156707, L-749329, Ro-47-0203, and A-127722 were 0.37, 0.29, 5.7, and 0.22 nM, resp. Addition of increasing doses of human serum albumin incrementally decreased the potency of the antagonists; in the presence of 5% of human serum albumin, the IC50 values increased to 62.8, 50.2, 122.7, and 6.72 nM for PD-156707, L-749329, Ro-47-0203, and A-127722, resp. In conclusion, ET and ET receptor antagonists exhibit a high degree of binding to plasma proteins, especially serum albumin. Consequently, serum albumin inhibits ET binding to its receptors, and also decreases the potency of ET receptor antagonists. Our findings may explain the discrepancy observed for ET receptor antagonists between in vitro and in vivo potencies.
IT 162412-70-6, PD-156707
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(endothelin and endothelin receptor antagonist binding to plasma proteins)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

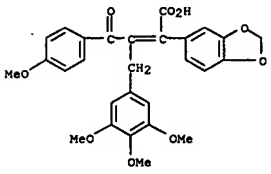
L4 ANSWER 111 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

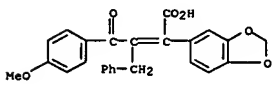
L4 ANSWER 112 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:253266 CAPLUS
DOCUMENT NUMBER: 124:331470
TITLE: Liquid chromatographic assay for a butenolide endothelin antagonist (PD 156707) in plasma
AUTHOR(S): Rossi, David T.; Hallak, Hussein; Bradford, Laura
CORPORATE SOURCE: Division of Warner Lambert Company, Parke-Davis Pharmaceutical Research, Ann Arbor, MI, 48105, USA
SOURCE: Journal of Chromatography, B: Biomedical Applications (1996), 677(2), 299-304
CODEN: JCBBEP; ISSN: 0378-4347
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A sensitive and selective liquid chromatog. assay for determining the non-peptide endothelin A receptor antagonist PD 156707 (I) in rat plasma has been developed and validated. The analyte was isolated from matrix by solid-phase extraction Liquid chromatog. separation was achieved isocratically on a 3.2 mm I.D., ODS column with a mobile phase of acetonitrile-ammonium phosphate (50 mM, pH 3.5) (44:56, volume/volume). Column effluent was monitored fluorometrically. Peak-height ratios (analyte/IS) were proportional to I concns. in rat plasma from 25 to 1000 ng/mL. Assay precision and accuracy for I, based on quality controls, was 9.5% relative standard deviation, with relative error of ±6.5%. The quantitation limit was 25 ng/mL for a 200-μL sample aliquot.
IT 162412-70-6, PD 156707
RL: ANT (Analyte); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(liquid chromatog. assay for a butenolide endothelin antagonist (PD 156707) in plasma)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 112 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

L4 ANSWER 113 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:228407 CAPLUS
DOCUMENT NUMBER: 124:332388
TITLE: Prevention of subarachnoid hemorrhage-induced cerebral vasospasm by oral administration of endothelin receptor antagonists
AUTHOR(S): Zuccarello, Mario; Soattin, Giovanni B.; Lewis, Adam I.; Breu, Volker; Hallak, Hussein; Rapoport, Robert M.
CORPORATE SOURCE: Department of Neurosurgery, University of Cincinnati, Cincinnati, OH, USA
SOURCE: Journal of Neurosurgery (1996), 84(3), 503-7
CODEN: JONSAC; ISSN: 0022-3085
PUBLISHER: American Association of Neurological Surgeons
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The purpose of this study was to investigate the effectiveness of oral treatment with the endothelin (ET)A/B receptor antagonist Ro 47-0203, 4-tert-butyl-N-[6-(hydroxy-ethoxy)-5-(2-methoxy-phenoxy)-2'-bipyrimidin-4-yl]-benzenesulfonamide (bosentan), and the ETA receptor antagonist 2-benzo[1,3]dioxol-5-yl-3-benzyl-4-(4-methoxy-phenyl)-4-oxobut-2-enoic acid monosodium salt (PD155080), in the prevention of subarachnoid hemorrhage (SAH)-induced delayed cerebral vasospasm. Double hemorrhage in the rabbit constricted the basilar artery to 34% of control as determined by angiog. Oral bosentan and PD155080 administration after the initial SAH decreased the magnitude of constriction to 9% and 16% of control, resp. Plasma and cerebrospinal fluid bosentan levels and plasma PD155080 levels were consistent with concns. reported to inhibit ET-1 constriction of blood vessels in vitro. These results support the use of oral administration of ETA/B and ETA receptor antagonists as potential specific treatment for vasospasm resulting from SAH in humans.
IT 162412-71-7, PD 155080
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(prevention of subarachnoid hemorrhage-induced cerebral vasospasm by oral administration of endothelin receptor antagonists)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

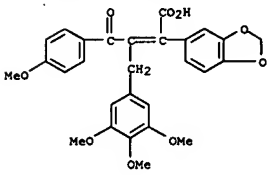


● Na

L4 ANSWER 113 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

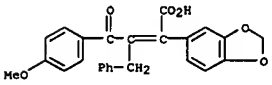
L4 ANSWER 114 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:966288 CAPLUS
DOCUMENT NUMBER: 124:45250
TITLE: Therapeutic potential of endothelin receptor antagonists in experimental stroke
AUTHOR(S): Patel, Toshal R.; Galbraith, Samuel L.; McAuley, Moira A.; Doherty, Annette M.; Graham, David I.; McCulloch, James
CORPORATE SOURCE: Wellcome Surgical Inst., Univ. of Glasgow, Glasgow, UK
SOURCE: Journal of Cardiovascular Pharmacology (1995), 26(Suppl. 3), S412-S415
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott-Raven
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This investigation demonstrates an increase in endothelin (ET)-mediated vascular tone in peri-ischemic areas after exptl. focal cerebral ischemia (middle cerebral artery occlusion) in the cat. Adventitial application of the butenolide antagonist PD155080 (30 μM), after MCA occlusions resulted in marked increases in caliber of dilated (10.6 ± 1.6% change from preinjection baseline) and constricted vessels (68.7 ± 17.5% change from preinjection baseline). Cerebral blood flow (measured by laser Doppler flowmetry) was reduced after MCA occlusion to 50% of preocclusion levels. I.v. administration of PD156707 30 min after MCA occlusion restored cerebral blood flow to preocclusion baseline levels at 6 h. The volume of ischemic damage in the cerebral hemisphere after MCA occlusion was significantly reduced (by 45%) after i.v. administration of PD156707.
IT 162412-70-6, PD156707 162412-71-7, PD 155080
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(therapeutic potential of endothelin receptor antagonists in exptl. stroke)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 114 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

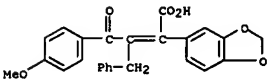
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

L4 ANSWER 115 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:966275 CAPLUS
DOCUMENT NUMBER: 124:528
TITLE: Potency of PD155080, an orally active ETA receptor antagonist, determined for human endothelin receptors
AUTHOR(S): Maguire, Janet J.; Kuc, Rhoda E.; Doherty, Annette M.; Davenport, Anthony P.
CORPORATE SOURCE: Addenbrooke's Hospital, University Cambridge, Cambridge, UK
SOURCE: Journal of Cardiovascular Pharmacology (1995), 26(Suppl. 3), S362-S364
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott-Raven
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors have determined, for the first time, the potency of a new ETA-selective endothelin (ET) antagonist, PD 155080, for human endothelin receptors. In sections of human left ventricle and human kidney PD 155080 competed for specific [125I]ET-1 binding with Kd values at the ETA receptor of 221.4 nM and 19.0 nM and at the ETB receptor of 86.5 μM and 17.7 μM. PD 155080 therefore has up to 1000-fold selectivity for the human ETA receptor. The ability of this compound to antagonize ET-1-mediated vasoconstriction was determined in human isolated coronary artery, saphenous vein, and left internal mammary artery. Increasing concns. of PD 155080 caused a progressive, parallel rightward shift of the ET-1 concentration-response curve without detrimental effect on the maximal response to ET-1. The pA2 values determined by Schild anal. were 6.87 in coronary artery, 6.75 in saphenous vein, and 7.25 in mammary artery. Slopes of the Schild regression lines were not significantly different from one, indicating a competitive mode of action. In addition, PD 155080 (1 μM) fully reversed the established contraction to ET-1 (30 nM) in saphenous vein. The potency of this compound is comparable to hat reported for the ETA-selective peptide antagonist BQ 123 [cyclo(D-Trp-L-Asp-L-Pro-D-Val-L-Leu)], which is effective in limiting tissue damage caused by ET-1 in animal models of pathol. vasospasm. PD 155080 may therefore be a good candidate for clin. use in diseases, such as subarachnoid hemorrhage, in which the ET system is implicated.
IT 162412-71-7, PD 155080
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(PD 155080 antagonistic potency and selectivity for human endothelin receptors)
RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 115 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

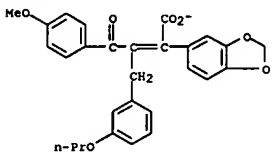
L4 ANSWER 116 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:966274 CAPLUS
DOCUMENT NUMBER: 124:83053
TITLE: Structure-activity relationships of a novel series of orally active nonpeptide ETA and ETA/B endothelin receptor-selective antagonists
AUTHOR(S): Doherty, Annette M.; Patt, William C.; Repine, Joseph; Edmunds, Jeremy J.; Berryman, Kent A.; Reisdorph, Billy R.; Walker, Donnelle M.; Haleen, Steven J.; Keiser, Joan A.; et al.
CORPORATE SOURCE: Departments Chemistry, Parke-Davis Pharmaceutical Research Division, Ann Arbor, MI, USA
SOURCE: Journal of Cardiovascular Pharmacology (1995), 26(Suppl. 3), S358-S361
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott-Raven
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The development of nonpeptide, low mol. weight antagonists with high potency, oral activity, and selectivity is an important objective to adequately define the potential role of endothelin (ET) and its isopeptides in human diseases. This report describes the structure-activity relationships, ETA/ETB selectivity, and pharmacokinetics of the PD 155080 and PD 156707 series of orally active nonpeptide ET receptor-selective antagonists. Modification of the substituents around the butenolide ring has led to compds. with differing selectivity for human ETA and ETB receptors. Thus, compds. with increased lipophilicity at R2 show increased ETB affinity and a more balanced ETA/ETB profile. For example, the 4-O-n-pentyl analog of PD 156707 is a potent competitive inhibitor of [125I]ET-1 and [125I]ET-3 binding to human cloned ETA and ETB receptors, with IC50s of 0.8 nM and 44 nM, resp. Pharmacokinetic properties can also be significantly influenced by structural modifications at the R2 group. The pharmacokinetics of PD 155719, PD 155080, and PD 156707 were compared in male Wistar rats after a 15 mg/kg i.v. or oral gavage dose (three animals per dose). Plasma concns. were determined by a specific HPLC assay. Oral bioavailability ranged from less than 55 for PD 155719 to 41% for PD 156707 and 87% for PD 155080.

IT 162412-70-6, PD 156707 162412-71-7, PD 155080
172519-47-0, PD 155719
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(structure-activity relationships of orally active nonpeptide ETA and ETA/B endothelin receptor-selective antagonists)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 116 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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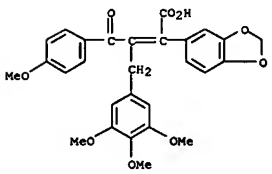
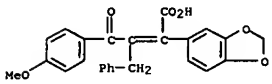
CRN 62-49-7
CMF C5 H14 N O

L4 ANSWER 116 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)



● Na

RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

RN 172519-47-0 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with α-[2-(4-methoxyphenyl)-2-oxo-1-[(3-propoxyphenyl)methyl]ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 172519-46-9
CMF C28 H25 O7

L4 ANSWER 117 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:957969 CAPLUS
DOCUMENT NUMBER: 124:29604
TITLE: An enantioselective process for the preparation of chiral triaryl derivatives and chiral intermediates for use therein
INVENTOR(S): Alexander, Rikki Peter; Warrellow, Graham John; Head, John Clifford; Boyd, Ewan Campbell; Porter, John Robert
PATENT ASSIGNEE(S): Celltech Therapeutics Ltd., UK
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9517386	A1	19950629	WO 1994-GB2799	19941222
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RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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GB 2299082	A	19960925	GB 1996-12213	19941222
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EP 736010	A1	19961009	EP 1995-903885	19941222
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JP 09510691	T	19971028	JP 1994-517279	19941222
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FI 9602599	A	19960620	FI 1996-2599	19960620
PRIORITY APPLN. INFO.:			GB 1993-26173 A	19931222
			WO 1994-GB2799 W	19941222

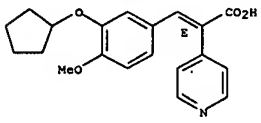
OTHER SOURCE(S): CASREACT 124:29604; MARPAT 124:29604
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB An enantioselective, multi-stage process is described, which uses as starting material an α,β-unsatd. olefin ArCH:C(R4)COAux [Ar, R4 = (independently) mono- or bicyclic (hetero)aryl; Aux = residue of chiral (R)- or (S)-isomeric auxiliary]. In the process, the olefins are converted to chiral triarylethanes ArCH(R3)CH2R4 [R4 defined as for Ar, R3], which are useful as PDE IV inhibitors (no data). A key step involves reaction of the olefins with an R3-containing organometallic reagent. The

L4 ANSWER 117 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
method can give isomers in high yield and e.e. of ≥ 98%, and is extendable to large-scale manuf. with e.e. of ≥ 95%. For example, condensation of 3-(cyclopentyloxy)-4-methoxybenzaldehyde with Et 4-pyridylacetate gave propenoate ester I, which underwent alk. hydrolysis,
conversion to the acid chloride, and imidation with the chiral auxiliary (2S)-bornane-10,2-sultam, to give key intermediate II. Reaction of II with PhMgBr, displacement of the auxiliary moiety with EtSH and BuLi, and sapon./decarbonylation of the resulting thiocarboxylate ester, gave target
enantiomer III.
IT 170985-16-7P 170985-51-0P 170985-56-5P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective preparation of chiral triarylethanes)
RN 170985-16-7 CAPLUS
CN 4-Pyridineacetic acid, α-[[3-(cyclopentyloxy)-4-methoxyphenyl]methylene]-, hydrochloride, (E)- (9CI) (CA INDEX NAME)

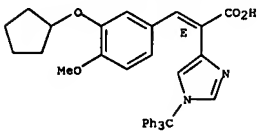
Double bond geometry as shown.



● HCl

RN 170985-51-0 CAPLUS
CN 1H-Imidazole-4-acetic acid, α-[[3-(cyclopentyloxy)-4-methoxyphenyl]methylene]-1-(triphenylmethyl)-, (E)- (9CI) (CA INDEX NAME)

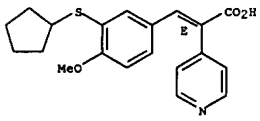
Double bond geometry as shown.



RN 170985-56-5 CAPLUS
CN 4-Pyridineacetic acid, α-[[3-(cyclopentylthio)-4-

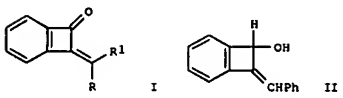
L4 ANSWER 117 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
methoxyphenyl]methylene]-, hydrochloride, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



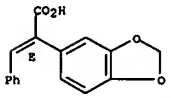
● HCl

L4 ANSWER 118 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:948027 CAPLUS
DOCUMENT NUMBER: 124:145542
TITLE: Base-catalyzed ring openings of benzocyclobutenones and -ols
AUTHOR(S): Bradley, J. C.; Durst, T.
CORPORATE SOURCE: Ottawa-Carleton Chem. Inst., Univ. Ottawa, Ottawa, ON,
K1N 6N5, Can.
SOURCE: Canadian Journal of Chemistry (1995), 73(10), 1660-5
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:145542
GI



AB The base-catalyzed ring opening of a number of isomeric E- and Z-benzylidenebenzocyclobutenones, e.g., I (R = Ph, R1 = H; R = H, R1 = Ph), and -ols, e.g., II, has been studied in both protic and aprotic solvents. Cleavage of the C1-C2 bond results in the formation of stilbenes with mainly, and at times exclusively, retained stereochem. For
the alcs., these results point to an oxyanion-induced carbon-carbon bond cleavage leading to a vinyl anion that is protonated with retention of configuration in the protic solvents rather than to an electrocyclic ring opening to an alkoxy o-quinodimethane. Reaction of the Z isomer of benzylidenebenzocyclobutenol with methyllithium in THF at 20° causes isomerization to the E isomer, cleavage of the C1-C2 bond, and recyclization of the resultant isomerized vinyl anion.
IT 77955-67-0P 77955-68-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ring cleavage of benzocyclobutenones and -ols)
RN 77955-67-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

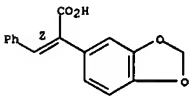
Double bond geometry as shown.



RN 77955-68-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-(phenylmethylene)-, (Z)- (9CI)

L4 ANSWER 118 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)

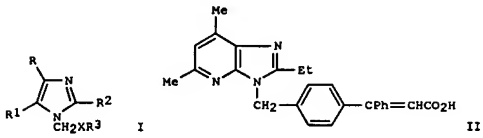
Double bond geometry as shown.



L4 ANSWER 119 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:946822 CAPLUS
DOCUMENT NUMBER: 123:340129
TITLE: New imidazopyridine derivatives as angiotensin II antagonists.
INVENTOR(S): Almansa, Carmen; Carceller, Elena; Gonzalez, Concepcion S.; Torres, M. Carmen; Bartroli, Javier
PATENT ASSIGNEE(S): Uriach, J., Spain; Cia, S. A.
SOURCE: Eur. Pat. Appl., 78 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 669333	A1	19950830	EP 1995-102658	19950224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
ES 2079315	A1	19960101	ES 1994-364	19940224
ES 2079315	B1	19961016		
CA 2143412	A1	19950825	CA 1995-2143412	19950223
NO 9500684	A	19950825	NO 1995-684	19950223
JP 07267951	A	19951017	JP 1995-61678	19950224
US 5554624	A	19960910	US 1995-393981	19950224
PRIORITY APPLN. INFO.:			ES 1994-364 A	19940224

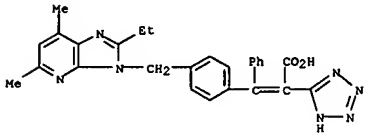
OTHER SOURCE(S): MARPAT 123:340129
GI



I II

AB Imidazopyridines I [RR1 = atoms required to complete a pyridine ring; X = C6H4, pyridylene; R2 = alkyl, cycloalkyl; R3 = substituted alkyl, alkenyl] (95 compds.) were prepared for use as angiotensin II antagonists (no data). Thus, CH2(OMe)2 was treated with EtO2CCH2P(O)(OEt)2 and 4-MeC6H4COPh to give Et 3-(4-methylphenyl)-3-phenyl-2-propenoate as a cis-trans mixture, which was converted to the bromomethyl compound and treated with 5,7-dimethyl-2-ethylimidazo[4,5-b]pyridine, followed by ester hydrolysis to give imidazopyridine II.
IT 170789-92-1P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

L4 ANSWER 119 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study); PREP (Preparation); USES (Uses)
(prepn. of imidazopyridine derivs. as angiotensin II antagonists)
RN 170789-92-1 CAPLUS
CN 1H-Tetrazole-5-acetic acid, α-[[4-[(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]phenylmethylene]- (9CI) (CA INDEX NAME)

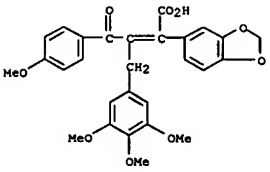


L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:896100 CAPLUS
DOCUMENT NUMBER: 123:313934
TITLE: Preparation of 2(5H)-furanones, 2(5H)-thiophenones, 2(5H)-pyrrolones and benzodioxolyls as endothelin antagonists
INVENTOR(S): Berryman, Kent Alan; Doherty, Annette Marian; Edmunds, Jeremy John; Patt, William Chester; Plummer, Mark Stephen; Repine, Joseph Thomas
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: PCT Int. Appl., 423 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

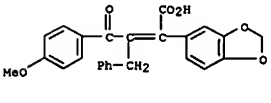
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9505376	A1	19950223	WO 1994-US9091	19940809
W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2165567	A1	19950223	CA 1994-2165567	19940809
AU 9475617	A	19950314	AU 1994-75617	19940809
AU 693110	B2	19980625		
EP 714391	A1	19960605	EP 1994-925831	19940809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 74179	A2	19961128	HU 1996-365	19940809
JP 09501920	T	19970225	JP 1994-507074	19940809
ZA 9406265	A	19960219	ZA 1994-6265	19940818
FI 9600671	A	19960419	FI 1996-671	19960214
NO 9600629	A	19960216	NO 1996-629	19960216
PRIORITY APPLN. INFO.:			US 1993-109751 A	19930819
			US 1994-217578 A	19940324
			US 1994-278882 A	19940726
			WO 1994-US9091 W	19940809

OTHER SOURCE(S): MARPAT 123:313934
AB Title compds. and salts thereof are prepared Chalcones were treated with KCN to give nitrile addition products, hydrolysis of which gave the corresponding acids which were then cyclized with aldehydes give 2(5H)-furanones. In vitro and in vivo antagonism was demonstrated. Title compds. are claimed for many human diseases in which endothelin is involved.
IT 162412-70-6P 162412-71-7P 169804-10-8P
169804-12-0P 169804-14-2P 169804-77-7P
169805-00-9P 169805-53-2P 169805-54-3P
169805-57-6P 169805-58-7P 169805-59-8P
169805-68-9P 169805-69-0P 169805-70-3P
169805-71-4P 169805-72-5P 169805-73-6P
169805-80-5P 169805-82-7P 169805-89-4P
169806-07-9P 169806-08-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 2(5H)-furanones, 2(5H)-thiophenones, 2(5H)-pyrrolones and benzodioxolyls as endothelin antagonists)
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



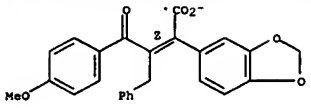
RN 169804-10-8 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 169804-09-5
CMF C25 H19 O6

Double bond geometry as shown.

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 62-49-7
CMF C5 H14 N O

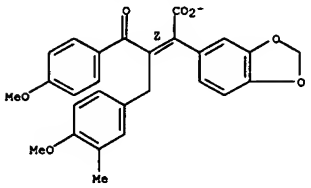
$Me_3{}^+N-CH_2-CH_2-OH$

RN 169804-12-0 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[1-[(4-methoxy-3-methylphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 169804-11-9
CMF C27 H23 O7

Double bond geometry as shown.

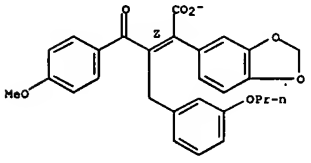


CM 2

CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N-CH_2-CH_2-OH$

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

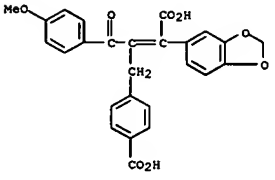


CM 2

CRN 62-49-7
CMF C5 H14 N O

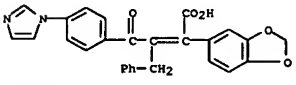
$Me_3{}^+N-CH_2-CH_2-OH$

RN 169805-00-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(4-carboxyphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, disodium salt (9CI) (CA INDEX NAME)



●2 Na

RN 169805-53-2 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-[4-(1H-imidazol-1-yl)phenyl]-2-oxo-1-(phenylmethyl)ethylidene]- (9CI) (CA INDEX NAME)



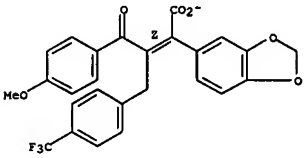
L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 169804-14-2 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[2-(4-methoxyphenyl)-2-oxo-1-[[4-(trifluoromethyl)phenyl]methyl]ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 169804-13-1
CMF C26 H18 F3 O6

Double bond geometry as shown.



CM 2

CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N-CH_2-CH_2-OH$

RN 169804-77-7 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with (Z)-α-[2-(4-methoxyphenyl)-2-oxo-1-[(3-propoxyphenyl)methyl]ethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

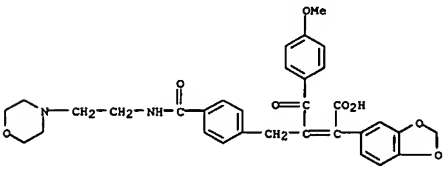
CM 1

CRN 169804-76-6
CMF C28 H25 O7

Double bond geometry as shown.

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

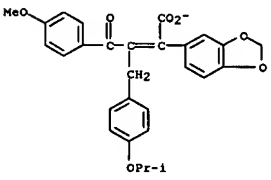
RN 169805-54-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[[4-[[[2-(4-morpholinyl)ethyl]amino]carbonyl]phenyl]methyl]-2-oxoethylidene]- (9CI) (CA INDEX NAME)



RN 169805-57-6 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with α-[2-(4-methoxyphenyl)-1-[[4-(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]-1,3-benzodioxole-5-acetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 169805-56-5
CMF C28 H25 O7



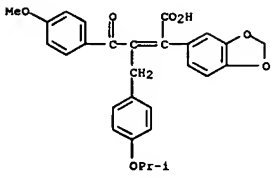
CM 2

CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N-CH_2-CH_2-OH$

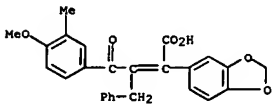
RN 169805-58-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[[4-(1-methylethoxy)phenyl]methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INDEX NAME)



● Na

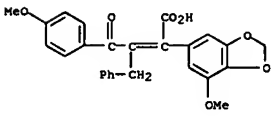
RN 169805-59-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

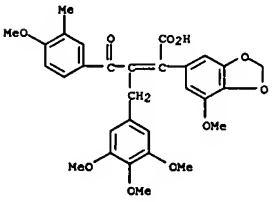
RN 169805-68-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[4-(acetylamino)phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, monopotassium salt (9CI) (CA INDEX
NAME)

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

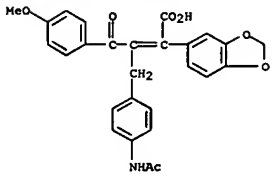
RN 169805-71-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium
salt (9CI) (CA INDEX NAME)



● Na

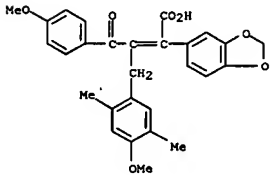
RN 169805-72-5 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● K

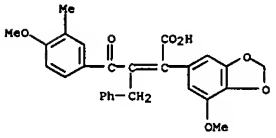
RN 169805-69-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[(4-methoxy-2,5-dimethylphenyl)methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

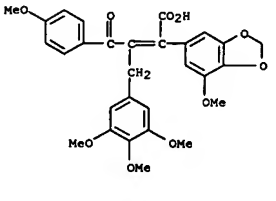
RN 169805-70-3 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

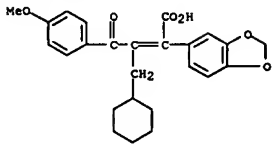
RN 169805-73-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, 7-methoxy-α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA
INDEX NAME)



● Na

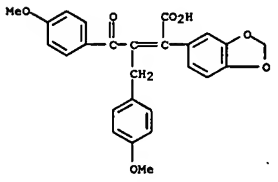
RN 169805-80-5 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-(cyclohexylmethyl)-2-(4-methoxyphenyl)-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

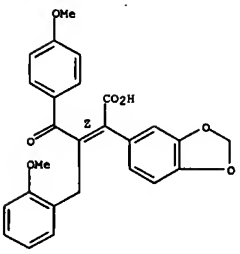
RN 169805-82-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(4-methoxyphenyl)methyl]-2-oxoethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

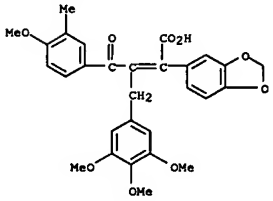
RN 169805-89-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxy-3-methylphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



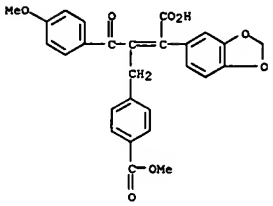
● Na

L4 ANSWER 120 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 169806-07-9 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[1-[[4-(methoxycarbonyl]phenyl]methyl]-2-(4-methoxyphenyl)-2-oxoethylidene]-, potassium salt (9CI) (CA INDEX NAME)



● K

RN 169806-08-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-1-[(2-methoxyphenyl]methyl]-2-oxoethylidene]-, sodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 121 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

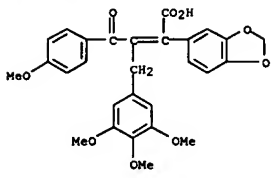
ACCESSION NUMBER: 1995:644396 CAPLUS
DOCUMENT NUMBER: 123:74514
TITLE: Pharmacological characterization of PD 156707, an orally active ETA receptor antagonist
AUTHOR(S): Reynolds, Elwood E.; Keiser, Joan A.; Haleen, Stephen J.; Walker, Donnelle M.; Olszewski, Bronislawa; Schroeder, Richard L.; Taylor, David G.; Hwang, Ok; Welch, Kathleen M.; et al.
CORPORATE SOURCE: Department Cardiovascular Therapeutics, Parke-Davis Pharmaceutical Research, Ann Arbor, MI, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1995), 273(3), 1410-17
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We describe the pharmacol. characteristics of PD 156707 (sodium 2-benzo[1,3]dioxol-5-yl-4-(4-methoxyphenyl)-4-oxo-3-(3,4,5-trimethoxybenzyl)but-2-enoate), a potent, orally active, nonpeptide antagonist of the endothelin A (ETA) receptor subtype. PD 156707 was designed on the basis of a compound identified by screening the Parke-Davis chemical library. PD 156707 is highly selective for the ETA receptor (ETAR) and inhibits the binding of [125I]-ET-1 to cloned human ETAR and ETBR with Ki values of 0.17 and 133.8 nM, resp. PD 156707 antagonizes ET-1-stimulated phosphoinositide hydrolysis in Ltk- cells expressing cloned human ETAR with an IC50 value of 2.4 nM. Pd 156707 inhibits vasoconstriction in isolated blood vessels mediated by ETAR (rabbit femoral artery) and ETBR (rabbit pulmonary artery) with pA2 values of 7.5 and 4.7, resp. PD 156707 administered orally to rats blocked subsequent ETAR-mediated pressor responses in vivo but had no effect on ETBR-mediated dilator responses. As a potent and orally active ETA-selective antagonist, PD 156707 will be useful in defining the physiol. and pathol. roles of ETAR.

IT 162412-70-6, PD 156707
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(pharmacol. characterization of PD 156707, an orally active ETA receptor antagonist)

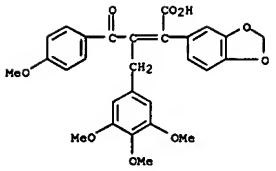
RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 121 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



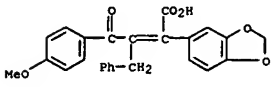
● Na

L4 ANSWER 122 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Na

RN 162412-71-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-(phenylmethyl)ethylidene]-, sodium salt (9CI) (CA INDEX NAME)



● Na

L4 ANSWER 122 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:481887 CAPLUS
DOCUMENT NUMBER: 122:230140
TITLE: Discovery of a Novel Series of Orally Active Non-Peptide Endothelin-A (ETA) Receptor-Selective Antagonists
AUTHOR(S): Doherty, Annette M.; Patt, William C.; Edmunds, Jeremy J.; Berryman, Kent A.; Reisdorph, Billy R.; Plummer, Mark S.; Shahripour, Aurash; Lee, Chet; Cheng, Xue-Min; et al.
CORPORATE SOURCE: Parke-Davis Pharmaceutical Research Div., Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (1995), 38(8), 1259-63
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:230140

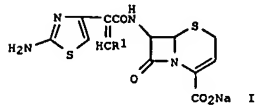
AB We have optimized the potency of an initial lead structure, PD 012527, to discover potent orally active ETA-selective antagonists, exemplified by PD 155080 (sodium 2-benzo[1,3]dioxol-5yl-3-benzyl-4-(4-methoxyphenyl)-4-oxobut-2-enoate) and PD 156707 (sodium 2-benzo[1,3]dioxo-5-yl-4-(4-methoxyphenyl)-4-oxo-3-(3,4,5-trimethoxybenzyl)-but-2-enoate). PD 155080 is a potent competitive inhibitor of [125I]ET-1 and [125I]ET-3 binding to human cloned ETA and ETB receptors with IC50's of 7.8 nM and 3.5 μM resp. The compound also antagonizes ET-1 induced arachidonic acid release in rabbit renal artery VSMC with an IC50 of 0.15 μM. PD 156707 is approx. 10-fold more potent in binding to human cloned ETA and ETB receptors with IC50s of 0.3 nM and 0.42 μM resp. and antagonizes ET-1 induced arachidonic acid release in rabbit renal artery VSMC with an IC50 of 1.1 nM.

IT 162412-70-6P, PD 156707 162412-71-7P, PD 155080
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and pharmacol. of nonpeptide endothelin A receptor antagonists)

RN 162412-70-6 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(4-methoxyphenyl)-2-oxo-1-[(3,4,5-trimethoxyphenyl)methyl]ethylidene]-, sodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 123 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:680438 CAPLUS
DOCUMENT NUMBER: 121:280438
TITLE: Synthesis and structural-activity relationships of 7β-[(Z)-2-(2-aminothiazol-4-yl)-3-(substituted)-2-propenoylamino[-3-desacetoxymethylcephalosporins
AUTHOR(S): Ishikura, Koji; Kubota, Tadatoshi; Minami, Kyoji; Hamashima, Yoshio; Nakashimizu, Hiromu; Motokawa, Kiyoshi; Yoshida, Tadashi
CORPORATE SOURCE: Shinogi Res. Lab., Shinogi and Co., Ltd., Osaka, 553, Japan
SOURCE: Journal of Antibiotics (1994), 47(4), 453-65
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

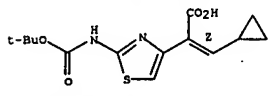


AB Synthesis and biol. activity of a series of 7β-[(Z)-2-(2-aminothiazol-4-yl)-3-(substituted) 2-propenoylamino]-3-cephem-4-carboxylic acids I (R1 = Me, Et, Pr, cyclopropyl, cyclohexylmethyl, etc.) and their pivaloyloxymethyl esters are described. These acid compds. exhibited potent antibacterial activity against both Gram-pos. and Gram-neg. bacteria. Pivaloyloxymethyl esters of selected compds. in this series were found to be well absorbed from small intestine in mice.

IT 114569-61-8P 158497-21-3P 158497-23-5P
158743-53-4P 158743-54-5P 158743-55-6P
158743-56-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of, with aminocephemcarboxylate)

RN 114569-61-8 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclopropylmethylene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

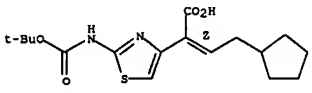
Double bond geometry as shown.



RN 158497-21-3 CAPLUS
CN 4-Thiazoleacetic acid, α-(2-cyclopentylethylidene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

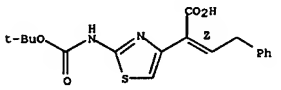
Double bond geometry as shown.

L4 ANSWER 123 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



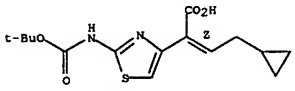
RN 158497-23-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-α-(2-phenylethylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



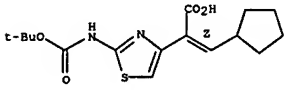
RN 158743-53-4 CAPLUS
CN 4-Thiazoleacetic acid, α-(2-cyclopropylethylidene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



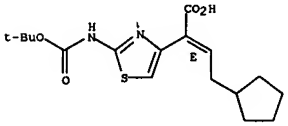
RN 158743-54-5 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclopentylmethylene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



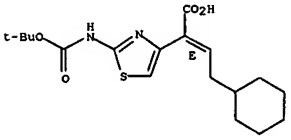
RN 158743-55-6 CAPLUS
CN 4-Thiazoleacetic acid, α-(2-cyclohexylethylidene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

L4 ANSWER 123 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



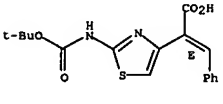
RN 159860-43-2 CAPLUS
CN 4-Thiazoleacetic acid, α-(2-cyclohexylethylidene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

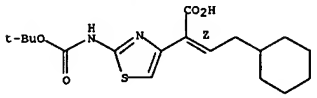


RN 159860-44-3 CAPLUS
CN 4-Thiazoleacetic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

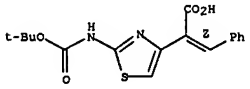


L4 ANSWER 123 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



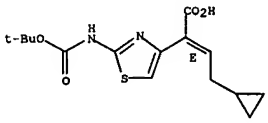
RN 158743-56-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-α-(phenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 159860-41-0P 159860-42-1P 159860-43-2P
159860-44-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 159860-41-0 CAPLUS
CN 4-Thiazoleacetic acid, α-(2-cyclopropylethylidene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

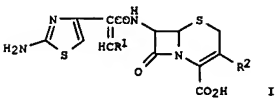


RN 159860-42-1 CAPLUS
CN 4-Thiazoleacetic acid, α-(2-cyclopentylethylidene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

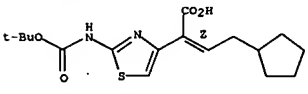
L4 ANSWER 124 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:655448 CAPLUS
DOCUMENT NUMBER: 121:255448
TITLE: Synthesis and structure-activity relationships of 7β-[(Z)-2-(2-aminothiazol-4-yl)-3-substituted) 2-propenolyamino]-3-cephems with C-3 substitutions
AUTHOR(S): Ishikura, Koji; Kubota, Tadashi; Minami, Kyoji; Hamashima, Yoshio; Nakashimizu, Hiromu; Motokawa, Kiyoshi; Kimura, Yasuo; Miwa, Hideaki; Yoshida, Tadashi
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan
SOURCE: Journal of Antibiotics (1994), 47(4), 466-76
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Synthesis and biol. activity of a series of 7β-[(Z)-2-(2-aminothiazol-4-yl)-3-(substituted) 2-propenoylamino]-3-cephem-4-carboxylic acids, e.g.,
I (R1 = Me, Et, cyclopentylmethyl, CH2SMe, CH2SPh, R2 = CH2OCOMe, Cl, CH2OMe, etc.), with C-3 substitutions and their pivaloyloxymethyl esters are described. These acid compds. exhibited potent antibacterial activity
against both Gram-pos. and Gram-neg. bacteria. Pivaloyloxymethyl esters of selected compds. in this series were found to be well absorbed from small intestine in mice. Pivaloyloxymethyl 7β-[(Z)-2-(2-aminothiazol-4-yl)-2-pentenoylamino]-3-carbamoyloxymethyl-3-cephem-4-carboxylate hydrochloride hydrate (S-1108) was finally selected as the candidate for clin. evaluation.
IT 158497-21-3 158497-23-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, with aminocephemcarboxylate)
RN 158497-21-3 CAPLUS
CN 4-Thiazoleacetic acid, α-(2-cyclopentylethylidene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

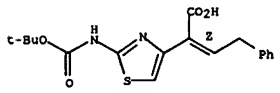
Double bond geometry as shown.



RN 158497-23-5 CAPLUS

L4 ANSWER 124 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 4-Thiazoleacetic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-α-(2-phenylethylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 125 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:579571 CAPLUS
DOCUMENT NUMBER: 121:179571
TITLE: preparation of isoxazole derivatives as lipoxygenase inhibitors
INVENTOR(S): Suzuki, Masahiro; Nozaki, Kenzi; Hosoya, Toshiyuki; Suzuki, Takashi; Basaki, Yuzi; Kozima, Mitiyo; Matsuura, Naosuke
PATENT ASSIGNEE(S): Taiho Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

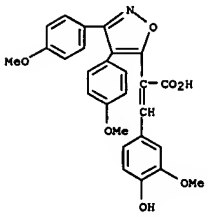
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9410157	A1	19940511	WO 1993-JP1572	19931029
W: AU, CA, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 06135948	A	19940517	JP 1992-333429	19921030
CA 2126972	A1	19940511	CA 1993-2126972	19931029
CA 2126972	C	19971223		
AU 9453450	A	19940524	AU 1994-53450	19931029
AU 671170	B2	19960815		
EP 623603	A1	19941109	EP 1993-923667	19931029
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5478856	A	19951226	US 1994-256058	19940627
PRIORITY APPLN. INFO.:			JP 1992-333429 A	19921030
			WO 1993-JP1572 W	19931029

OTHER SOURCE(S): MARPAT 121:179571
GI

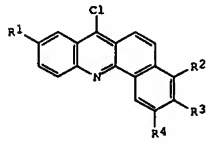
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Isoxazole derivs. [I; R1, R2 = H, alkyl, alkoxy, halo; R3 = OH. alkyl, alkoxy, acyl, etc.; X = bond, N(Z)CO (wherein Z = H, alkyl, carboxyalkyl, etc.); Y = (un)substituted CH:CH, CH:CHCH:CH; m, n = 0-5] are prepared and formulated. A mixture of isoxazole derivative II, cinnamic acid derivative III, 1-hydroxybenzotriazole, and DCC in DMF was stirred at room temperature to give 50.6% IV, which showed IC50 of 2.87 μM and 1.17 μM against cyclooxygenase and lipoxygenase, resp. Granular, tablet, capsule, injection, and syrup formulations were given.
IT 157724-69-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

L4 ANSWER 125 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as lipoxygenase inhibitor)
RN 157724-69-1 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3-methoxyphenyl)methylene]-3,4-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

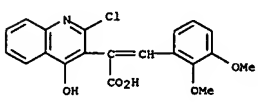


L4 ANSWER 126 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:533931 CAPLUS
DOCUMENT NUMBER: 121:133931
TITLE: A photochemical synthesis of benzo[c]acridines
AUTHOR(S): Suresh, J. R.; Jayabalan, L.; Shanmugam, P.
CORPORATE SOURCE: Dep. Chem., Bharathiar Univ., Coimbatore, 641 046, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1994), 33B(1), 79-84
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:133931
GI



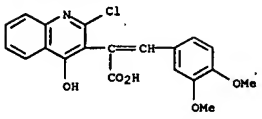
I

AB A photochem. preparation of several derivs. of benzo[c]acridines I (R1 = H, Me, Br; R2 = H, Cl, OMe; R3, R4 = H, OMe) using substituted 3-styryl-4-quinolinones as precursors is described. The precursors are obtained by condensation of 4-hydroxy-2-quinolinone-3-acetic acids with benzaldehydes.
IT 157192-36-4P 157192-37-5P 157192-38-6P
157192-39-7P 157192-40-0P 157192-41-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for benzo[c]acridine)
RN 157192-36-4 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-α-[(2,3-dimethoxyphenyl)methylene]-4-hydroxy- (9CI) (CA INDEX NAME)

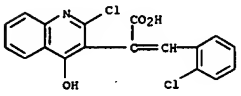


RN 157192-37-5 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-α-[(3,4-dimethoxyphenyl)methylene]-4-hydroxy- (9CI) (CA INDEX NAME)

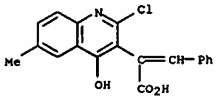
L4 ANSWER 126 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



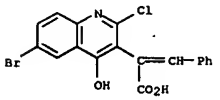
RN 157192-38-6 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-α-[(2-chlorophenyl)methylene]-4-hydroxy- (9CI) (CA INDEX NAME)



RN 157192-39-7 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-4-hydroxy-6-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

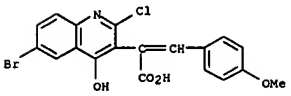


RN 157192-40-0 CAPLUS
CN 3-Quinolineacetic acid, 6-bromo-2-chloro-4-hydroxy-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



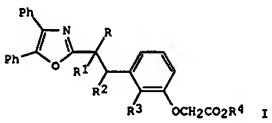
RN 157192-41-1 CAPLUS
CN 3-Quinolineacetic acid, 6-bromo-2-chloro-4-hydroxy-α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 126 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 127 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:106838 CAPLUS
DOCUMENT NUMBER: 120:106838
TITLE: Nonprostanoid prostacyclin mimetics. 4. Derivatives of 2-[3-[2-(4,5-diphenyl-2-oxazolyl)ethyl]phenoxy]acetic acid substituted α to the oxazole ring
AUTHOR(S): Meanwell, Nicholas A.; Rosenfeld, Michael J.; Wright, J. J. Kim; Brassard, Catherine L.; Buchanan, John O.; Federici, Marianne E.; Fleming, J. Stuart; Gamberdella, Marianne; Hartl, Karen S.; et al.
CORPORATE SOURCE: Div. Chem., Bristol-Myers Squibb Pharm. Res. Inst., Wallingford, CT, 06492-7660, USA
SOURCE: Journal of Medicinal Chemistry (1993), 36(24), 3871-83
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:106838
GI



AB Title compds. I [R = H, CO2H, esterified CO2H, CONH2, substituted CONH2, CN, P(O)(OEt)2, S(O)nMe (n = 0-2), alkyl, Ph, hydroxyalkyl; R1R2 = H2, bond; R1 = allyl, R2 = H; R3 = H, OMe; R4 = H, Me, CMe3, Na] were synthesized and evaluated as inhibitors of ADP-induced aggregation of human platelets in vitro. I (R = CO2Et, R1R2 = bond, R3, R4 = H), evaluated as an equal mixture of geometrical isomers, inhibited platelet aggregation with an IC50 of 0.36 μM. Evaluation of the individual Me ester derivs. revealed that (E)-I (R = CO2Et, R1R2 = bond, R3 = H, R4 = Me) was 10-fold more potent than (Z)-I (R = CO2Et, R1R2 = bond, R3 = H, R4 = Me). I (R = CO2Me, R1-R4 = H) inhibited platelet aggregation with an IC50 of 0.08 μM, 15-fold more potent than the unsubstituted prototype I (R-R4 = H). I (R = CO2Et, CO2CHMe2, R1-R4 = H) were less effective as were I (R = CO2H, R1-R4 = H) and a series of amides. None of the other I (R ≠ H, R1-R4 = H) were significantly more potent inhibitors of platelet function than I (R-R4 = H). The results indicate the presence of a pocket in the PGI2 receptor protein that preferentially recognizes small, polar but uncharged substituents. The structure-activity correlates are suggestive of a hydrogen-bond interaction between a donor moiety on the PGI2 receptor and the methoxycarbonyl functionality of I (R = CO2Me, R1-R4 = H) that is sensitive to both the size of the substituent and its stereochem. presentation in this structural class of PGI2 mimetics. I (R = CO2Et, R1-R4 = H) dose-dependently displaced [3H]iloprost from human platelet membranes and stimulated adenylate cyclase. However, the maximal stimulation was less than that recorded for

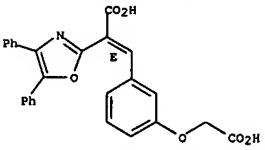
L4 ANSWER 127 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

iloprost, indicating that I (R = CO2Et, R1-R4 = H) functions as a partial agonist at the PGI2 receptor.

IT 147593-97-3 147593-98-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation as prostacyclin mimetic)

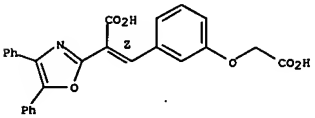
RN 147593-97-3 CAPLUS
CN 2-Oxazoleacetic acid, α-[[3-(carboxymethoxy)phenyl]methylene]-4,5-diphenyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



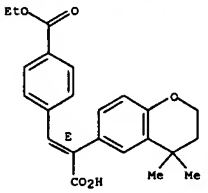
RN 147593-98-4 CAPLUS
CN 2-Oxazoleacetic acid, α-[[3-(carboxymethoxy)phenyl]methylene]-4,5-diphenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

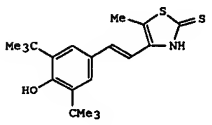


L4 ANSWER 128 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:625781 CAPLUS
DOCUMENT NUMBER: 119:225781
TITLE: Synthesis of potential metabolites of ethyl (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzopyran-6-yl)-1-propenyl]benzoate
AUTHOR(S): Sunthankar, P. S.; Berlin, K. D.; Nelson, Eldon C.; Thorne, R. Lori; Geno, Paul W.; Archer, Jeffrey C.; Rolf, Lester L., Jr.; Bartels, Kenneth E.
CORPORATE SOURCE: Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
SOURCE: Journal of Pharmaceutical Sciences (1993), 82(5), 543-5
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Potential metabolites of the title compound (I) were synthesized. The new
compds. include dihydrodimethylbenzopyrans II [R = (E)-CMe:CHCO2Et, (E)-CMe:CHCO2H, CO2H, Q, (E)-HOCH2C:CHC6H4CO2Et-4, (E)-OCHC:CHC6H4CO2Et-4,
(E)-HO2CC:CHC6H4CO2Et-4]. Stereospecific oxidizing reagents and/or conditions were developed for these sensitive systems and include the use of SeO2, Clorox bleach, activated MnO2, and NaClO2 in the presence of resorcinol as a chlorine scavenger.
IT 150799-40-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 150799-40-9 CAPLUS
CN 2H-1-Benzopyran-6-acetic acid, α-[[4-(ethoxycarbonyl)phenyl]methylene]-3,4-dihydro-4,4-dimethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



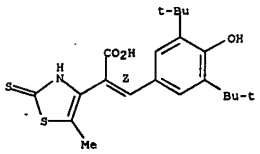
L4 ANSWER 129 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:603340 CAPLUS
DOCUMENT NUMBER: 119:203340
TITLE: Synthesis and transformations of 2,6-bis(1,1-dimethylethyl)-4-[2-(thiazolyl)ethenyl]phenols
AUTHOR(S): Unangst, Paul C.; Connor, David T.
CORPORATE SOURCE: Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Heterocyclic Chemistry (1992), 29(5), 1097-100
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:203340
GI



I

AB (Thiazolylethenyl)phenols, e.g., I, were prepared as potential antiinflammatories by reaction of thiazole-4- and 5-acetic acid derivs. with 3,5-di-tert-butyl-4-hydroxybenzaldehyde. Alternatively, an arylethenyl Me ketone was brominated and the bromoketone product reacted with Me dithiocarbamate, ammonium dithiocarbamate, or thiourea.
IT 150535-76-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)
RN 150535-76-5 CAPLUS
CN 4-Thiazoleacetic acid, α-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]-2,3-dihydro-5-methyl-2-thioxo-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

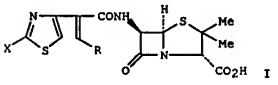


L4 ANSWER 129 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 130 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:449143 CAPLUS
DOCUMENT NUMBER: 119:49143
TITLE: Preparation of (hetero)polycycloalkyl-substituted acrylamido-penicillanic acid derivatives as antibacterials
INVENTOR(S): Ponsford, Roger John; Stachulski, Andrew Valentine
PATENT ASSIGNEE(S): SmithKline Beecham PLC, UK
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9304070	A1	19930304	WO 1992-GB1484	19920810
W: AU, CA, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
AU 9223992	A	19930316	AU 1992-23992	19920810
PRIORITY APPLN. INFO.:			GB 1991-17783 A	19910817
			WO 1992-GB1484 A	19920810

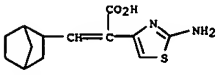
OTHER SOURCE(S): MARPAT 119:49143
GI



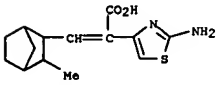
I

AB Title compds. [I; X = H, NHR1; R = (substituted) spiro, fused, or bridged bicyclic or tricyclic group optionally containing ≥1 of O, N, and S; R1 = H, protecting group], and salts or in-vivo hydrolyzeable esters thereof,
were prepared for treatment of bacterial infections (no data). Thus, Z-[2-(2-aminothiazol-4-yl)-3-(bicyclo[2.2.1]hept-2-yl)]propenoic acid (preparation from 2-norbornenemethanol and Me 2-acetamidothiazol-4-yl-acetate
given) was stirred with 1-hydroxytriazole and DCC in THF at 0°; the mixture (containing active ester) was added to 6-aminopenicillanic acid in 1N
NaOH to give Na 6β-[[Z-2-(2-aminothiazol-4-yl)-3-(bicyclo[2.2.1]hept-2-yl)]propenamido]penicillanate.
IT 135577-08-1P 135577-29-6P 135577-38-7P
135577-39-8P 135577-43-4P 135577-46-7P
135577-49-0P 135637-88-6P 148431-00-9P
148431-03-2P 148496-92-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for substituted acrylamidopenicillanic acid
antibacterial)
RN 135577-08-1 CAPLUS

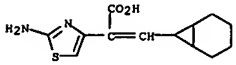
L4 ANSWER 130 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.1]hept-2-ylmethylene)-, [1α,2β(Z),4α]- (9CI) (CA INDEX NAME)



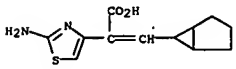
RN 135577-29-6 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(3-methylbicyclo[2.2.1]hept-2-yl)methylene]- (9CI) (CA INDEX NAME)



RN 135577-38-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[4.1.0]hept-7-ylmethylene)-, [1α,6α,7α(Z)]- (9CI) (CA INDEX NAME)

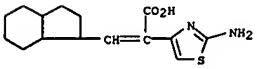


RN 135577-39-8 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[3.1.0]hex-6-ylmethylene)-, [1α,5α,6α(Z)]- (9CI) (CA INDEX NAME)

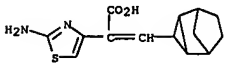


RN 135577-43-4 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(1-methoxybicyclo[2.2.2]oct-5-en-2-yl)methylene]-, [1α,2β(Z),4β]- (9CI) (CA INDEX NAME)

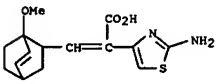
L4 ANSWER 130 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



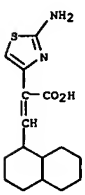
RN 148431-03-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(tricyclo[3.2.1.02,4]oct-3-ylmethylene)-, [1α,2β,3α(Z),4β,5α]- (9CI) (CA INDEX NAME)



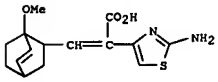
RN 148496-92-8 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(1-methoxybicyclo[2.2.2]oct-5-en-2-yl)methylene]-, [1α,2α(Z),4β]- (9CI) (CA INDEX NAME)



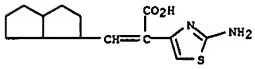
IT 135577-31-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for substituted acrylamidopenillanic acid derivative)
RN 135577-31-0 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(decahydro-1-naphthalenyl)methylene]- (9CI) (CA INDEX NAME)



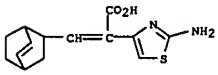
L4 ANSWER 130 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



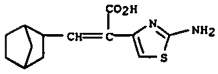
RN 135577-46-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(octahydro-1-pentalenyl)methylene]- (9CI) (CA INDEX NAME)



RN 135577-49-0 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.2]oct-5-en-2-ylmethylene)-, [1α,2α(Z),4α]- (9CI) (CA INDEX NAME)



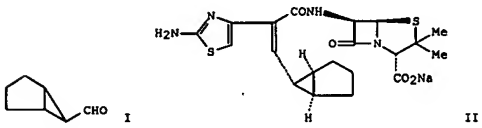
RN 135637-88-6 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.1]hept-2-ylmethylene)-, [1α,2α(Z),4α]- (9CI) (CA INDEX NAME)



RN 148431-00-9 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(octahydro-1H-inden-1-yl)methylene]- (9CI) (CA INDEX NAME)

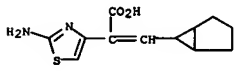
L4 ANSWER 130 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 131 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:427863 CAPLUS
DOCUMENT NUMBER: 119:27863
TITLE: Stereoselective synthesis of BRL 56173, a bicyclic acrylic penicillin highly stable to β-lactamases
AUTHOR(S): Atkins, Richard J.; Ponsford, Roger J.; Stachulski, Andrew V.
CORPORATE SOURCE: Dep. Synth. Chem., SmithKline Beecham Pharm., Leigh/Tonbridge/Kent, TN119AN, UK
SOURCE: Journal of Antibiotics (1993), 46(2), 362-5
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

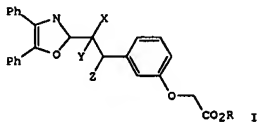
AB Exo-Bicyclohexanecarboxaldehyde I was efficiently prepared by peracetic acid
oxidation of norbornadiene to give an exo-bicyclohexenecarboxaldehyde followed epimerization and hydrogenation. I was then elaborated to the title compound (II). The bactericidal activity of II is also reported.
IT 135577-39-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 135577-39-8 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[3.1.0]hex-6-ylmethylene)-, (1α,5α,6α(Z))- (9CI) (CA INDEX NAME)



L4 ANSWER 132 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:254920 CAPLUS
DOCUMENT NUMBER: 118:254920
TITLE: Oxazole carboxylic acid derivatives
INVENTOR(S): Meanwell, Nicholas A.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: U.S., 18 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5187188	A	19930216	US 1992-862674	19920403
PRIORITY APPLN. INFO.:			US 1992-862674	19920403

OTHER SOURCE(S): MARPAT 118:254920
GI

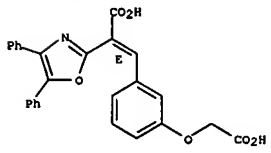


I

AB A novel series of oxazole derivs. I (X = CN, CO2R1, CONR2R3; Y = H, Z = H;
YZ = bond; R, R1 = H, Na, C1-5 alkyl R2, R3 = H, C1-5 alkyl] were prepared
and evaluated as human platelet aggregation inhibitors. I are thus useful
as inhibitors of ADP-induced blood platelet aggregation in humans.
IT 147593-97-3P 147593-98-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and blood platelet aggregation inhibition by)
RN 147593-97-3 CAPLUS
CN 2-Oxazoleacetic acid, α-[[3-(carboxymethoxy)phenyl]methylene]-4,5-diphenyl-, (E)- (9CI) (CA INDEX NAME)

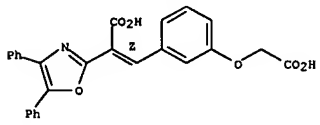
Double bond geometry as shown.

L4 ANSWER 132 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

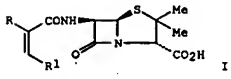


RN 147593-98-4 CAPLUS
CN 2-Oxazoleacetic acid, α-[[3-(carboxymethoxy)phenyl]methylene]-4,5-diphenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



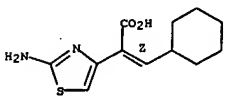
L4 ANSWER 133 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:254591 CAPLUS
DOCUMENT NUMBER: 118:254591
TITLE: Synthesis and structure-activity relationships of some
6β-acrylamido penicillins
AUTHOR(S): Anderson, Richard K.; Chapman, Pauline C.; Cosham, Suzanne c.; Davies, J. Sydney; Grinter, Trevor J.; Harris, Michael A.; Merrikin, David J.; Mitchell, Christina A.; Ponsford, Roger J.; et al.
CORPORATE SOURCE: SmithKline Beecham Pharmaceuticals Research and Development, Betchworth/Surrey, RH3 7AJ, UK
SOURCE: Journal of Antibiotics (1993), 46(2), 331-42
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Syntheses are described for the title compds. I (R = 2-aminothiazol-4-yl, R1 = Ph, Me3C, Me3CCH2, cycloalkyl, 4-tetrahydropyranyl, 4-tetrahydrothiapyranyl; R = 4-thiazolyl, 2-thienyl, R1 = cyclohexyl). In
vitro results for these compds. against a range of Gram-pos. and Gram-neg.
bacteria showed in most cases good stability against both penicillinase and TEM-1 β-lactamase. I (R = 2-aminothiazol-4-yl) showed the best intrinsic activity, I (R = 2-aminothiazol-4-yl, R1 = cyclohexyl) (II) being the most promising. The 1-acetoxyethyl ester of II was also prepared
and in exptl. animal studies the in vivo properties of this compound compared favorably with cefuroxime axetil. These results are reported together with selected in vivo data for the other compds.
IT 126781-75-7P 126781-80-4P 126781-81-5P
147699-50-1P 147699-51-2P 147699-55-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of, with aminopenicillanic acid)
RN 126781-75-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(cyclohexylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

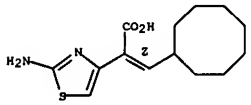
Double bond geometry as shown.



L4 ANSWER 133 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

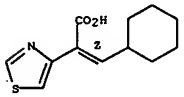
RN 126781-80-4 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(cyclooctylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



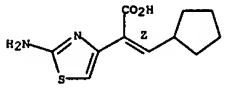
RN 126781-81-5 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclohexylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 147699-50-1 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(cyclopentylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

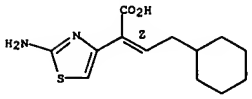
Double bond geometry as shown.



RN 147699-51-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(2-cyclohexylethylidene)-, (Z)- (9CI) (CA INDEX NAME)

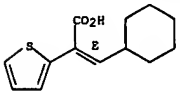
Double bond geometry as shown.

L4 ANSWER 133 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 147699-55-6 CAPLUS
CN 2-Thiopheneacetic acid, α-(cyclohexylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

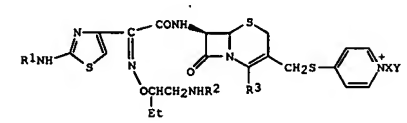


L4 ANSWER 134 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

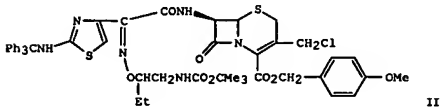
ACCESSION NUMBER: 1993:124297 CAPLUS
DOCUMENT NUMBER: 118:124297
TITLE: Preparation of cephalosporin compounds
INVENTOR(S): Kogami, Yuji; Sakurai, Kanako; Honda, Eiichi; Yamashita, Akitake; Watanabe, Hideyuki; Yaso, Masao
PATENT ASSIGNEE(S): Toyo Jozo Co., Ltd., Japan; Kyoto Pharmaceutical Industries, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE.	APPLICATION NO.	DATE
JP 04221388	A	19920811	JP 1990-411880	19901220
PRIORITY APPLN. INFO.:			JP 1990-411880	19901220

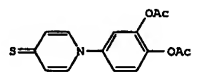
OTHER SOURCE(S): MARPAT 118:124297
GI



I



II



III

AB Cephalosporin derivs. [I; R1, R2 = H, protecting group; R3 = CO2-, (protected) CO2H; X = (CH2)n (wherein n = 0, 1, 2), CR4:CH (wherein R4 = H, CO2-, ester residue, etc.); Y = (protected) hydroxy-substituted Ph, (oxo)pyridyl, etc.], especially effective against gram-pos., gram-neg., and other Pseudomonas microbes, are prepared NaI was added to a solution of syn-II in DMF with stirring at 5-10° under Ar, thione III was added with stirring at 5-10°, H2O was added, the precipitate was filtered, washed, re-dissolved in CHCl3, dried with MgSO4, filtered, and the filtrate was concentrated in vacuo to give the iodide precursor, which was dissolved in PhOMe

L4 ANSWER 134 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

and the soln. was stirred with CF3CO2H at 0-5° to give 93.6% I.CF3CO2H [R1 = R2 = H, R3 = CO2-, XY = 3,4-(AcO)2C6H3], which showed MIC of 0.78 μg/mL against Staphylococcus aureus FDA209P, 0.10 μg/mL against Escherichia coli NIHJ JC-2, etc.

IT 146287-93-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as bactericide)

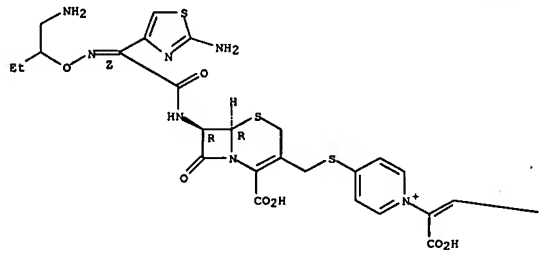
RN 146287-93-6 CAPLUS
CN Pyridinium, 4-[[[7-[[[[1-(aminomethyl)propoxy]imino](2-amino-4-thiazolyl)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]thio]-1-[1-carboxy-2-(3,4-dihydroxyphenyl)ethenyl]-, [6R-[6α,7β(Z)]]-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 146287-92-5
CMF C31 H32 N7 O9 S3

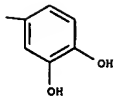
Absolute stereochemistry.
Double bond geometry as described by E or Z.

PAGE 1-A



L4 ANSWER 134 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B

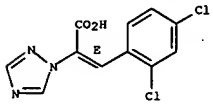


CM 2

CRN 14477-72-6
CMF C2 F3 O2

L4 ANSWER 135 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:647064 CAPLUS
DOCUMENT NUMBER: 117:247064
TITLE: Photochemical transformation of (E)-1-(2,4-dichlorophenyl)-4,4 dimethyl-2-(1,2,4-triazol-1-yl)-7-penten-3-ol)
AUTHOR(S): Dureja, P.; Walia, S.
CORPORATE SOURCE: Div. Agric. Chem., IARI, New Delhi, 110012, India
SOURCE: Toxicological and Environmental Chemistry (1992), 36(1-2), 15-21
CODEN: TECSDY; ISSN: 0277-2248
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Photodegrdn. of diniconazole (E)-1-(2,4-dichlorophenyl)-4-dimethyl-2-(1,2,4-triazol-1-yl)-7-penten-3-ol) in methanol, as a thin film, and on soil surface under UV light and sunlight was investigated. Irradiation of diniconazole (E) in methanol yielded, in addition to minor DTP-acid (E) and (Z) and DTP-aldehyde (E) and (Z), the major (Z)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)-7 penten-3-one. When applied on glass thin-layer plates, diniconazole was quickly dissipated with a half life of 2 h under UV light and 2.5 days in sunlight.
IT 144759-51-3 144759-52-4
RL: BIOL (Biological study)
(diniconazole photodegrdn. product)
RN 144759-51-3 CAPLUS
CN 1H-1,2,4-Triazole-1-acetic acid, α-[(2,4-dichlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

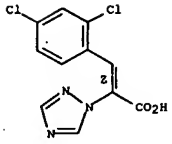
Double bond geometry as shown.



RN 144759-52-4 CAPLUS
CN 1H-1,2,4-Triazole-1-acetic acid, α-[(2,4-dichlorophenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

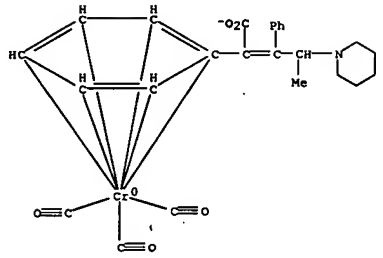
L4 ANSWER 135 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 136 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:591985 CAPLUS
DOCUMENT NUMBER: 117:191985
TITLE: Reaction of aminocarbene complexes of chromium with alkynes. 1. Formation and rearrangement of ketene and nitrogen ylide complexes
AUTHOR(S): Chelain, Evelyne; Goumont, Regis; Hamon, Louis; Parlier, Andree; Rudler, Michele; Rudler, Henri; Daran, Jean Claude; Vaissermann, Jacqueline
CORPORATE SOURCE: Lab. Chim. Org., Univ. Pierre et Marie Curie, Paris, 75252, Fr.
SOURCE: Journal of the American Chemical Society (1992), 114(21), 8088-98
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:191985
AB The title reactions of chromium-containing carbene complexes (CO)5Cr:C(R1)N(R2R3) [R1 = H, Me, Ph; R2 = Me; R3 = Me, cyclopropyl, cyclopropylmethyl; R2R3 = (CH2)5] 8 and (CO)5Cr:C[(CH2)3C.tplbond.CPh]N(R1 R2) [R1 = R2 = Me; R1R2 = (CH2)5, (CH2)4] 9, bearing alkyl groups of low migratory aptitude on nitrogen were examined In contrast to complexes in which nitrogen bears either an alkyl and an allyl or a benzyl group or is part of a strained cycle, which give heterocycles upon alkyne/CO insertions followed by nitrogen-to-carbon migrations, complexes 8 and 9 lead to stable nitrogen ylides, which could be fully characterized by x-ray crystallog. in the case of 8 [R1 = H, R2R3 = (CH2)5] and 9 [R1 = R2 = Me). Moreover, in the case of complexes of the general structure 9, ketene precursors of the ylides could either be detected (R1 = Me, R2 = CH2Ph) or isolated and characterized [R2R3 = (CH2)5]. The new ylide complexes undergo, upon moderate heating, Stevens-type rearrangements to the expected heterocyclic compds. as a result of nitrogen-to-carbon migrations of various alkyl groups, and upon treatment with dimethyldioxirane, they undergo oxidation to lactone complexes.
IT 131374-61-3P 131374-63-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 131374-61-3 CAPLUS
CN Chromate(1-), tricarbonyl[(1,2,3,4,5,6-η)-α-[(1E)-1-phenyl-2-(1-piperidinyl)propylidene]benzeneacetato]-, hydrogen (9CI) (CA INDEX NAME)

L4 ANSWER 136 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

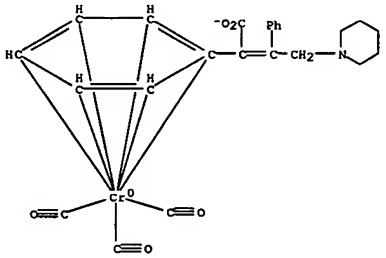


PAGE 2-A

● H^+

RN 131374-63-5 CAPLUS
CN Chromate(1-), tricarbonyl[(1,2,3,4,5,6-η)-α-[(1E)-1-phenyl-2-(1-piperidinyl)ethylidene]benzeneacetato]-, hydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



L4 ANSWER 136 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 2-A

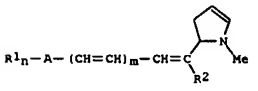
● H^+

L4 ANSWER 137 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:581390 CAPLUS
DOCUMENT NUMBER: 117:181390
TITLE: Nonlinear optical methylpyrrole derivative material
INVENTOR(S): Nakamura, Satoshi; Imahashi, Satoshi
PATENT ASSIGNEE(S): Toyobo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

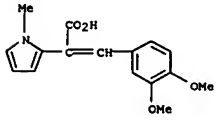
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04161932	A	19920605	JP 1990-288108	19901024
PRIORITY APPLN. INFO.:			JP 1990-288108	19901024

GI



I

AB The material consists of N-methylpyrrole derivative I (R1 = aromatic hydrocarbon group, heterocyclic group; R1 = amino, cyclic amino, alkyl, alkoxy, mercaptoalkoxy, halo, carboxyl, alkoxycarbonyl, C1-12-containing alkanoyloxy, nitro, cyano, alkanoylamide; R2 = cyano, carboxyl, alkoxycarbonyl, amide; m = 0-3; n = 0-5). The material showed high 2nd harmonic generation and good storage stability.
IT 143650-19-5P
RL: TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(nonlinear optical material, with high second harmonic generation and storage stability)
RN 143650-19-5 CAPLUS
CN 1H-Pyrrole-2-acetic acid, α-[(3,4-dimethoxyphenyl)methylene]-1-methyl- (9CI) (CA INDEX NAME)

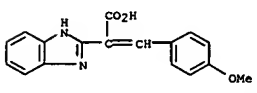


L4 ANSWER 138 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

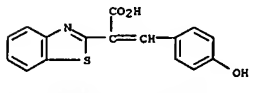
ACCESSION NUMBER: 1992:500666 CAPLUS
DOCUMENT NUMBER: 117:100666
TITLE: Nonlinear optical materials
INVENTOR(S): Nakamura, Satoshi; Imahashi, Satoshi
PATENT ASSIGNEE(S): Toyo Boseki K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04040429	A	19920210	JP 1990-149378	19900606
PRIORITY APPLN. INFO.:			JP 1990-149378	19900606

OTHER SOURCE(S): MARPAT 117:100666
AB The material contains I (R1=amino group optionally substituted by C1-18 radical(s), ring amino group, alkyl or alkoxy group optionally substituted by halogen, or mercaptoalkoxy, acylamide, ester, thioester, OH, mercaptohydroxyl, or halogen radical, or electron-attracting group, l=1-5; R2=organic group different from or same with R1 or halogen, m=0-3, n=0-4; Ring A=aromatic or heteroarom.; X=N, O, and/or S; Y=H, CN, COOH, carboxylic acid ester, or NO2).
IT 142885-23-2 142885-73-2 142885-74-3
142885-76-5 142885-77-6 142885-78-7
142885-79-8 142885-80-1 142885-81-2
142885-82-3 142885-83-4
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(nonlinear optical materials from)
RN 142885-23-2 CAPLUS
CN 1H-Benzimidazole-2-acetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

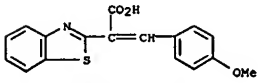


RN 142885-73-2 CAPLUS
CN 2-Benzothiazoleacetic acid, α-[(4-hydroxyphenyl)methylene]- (9CI) (CA INDEX NAME)

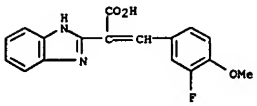


RN 142885-74-3 CAPLUS

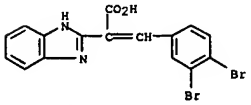
L4 ANSWER 138 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Benzothiazoleacetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



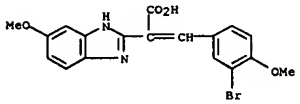
RN 142885-76-5 CAPLUS
CN 1H-Benzimidazole-2-acetic acid, α-[(3-fluoro-4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 142885-77-6 CAPLUS
CN 1H-Benzimidazole-2-acetic acid, α-[(3,4-dibromophenyl)methylene]- (9CI) (CA INDEX NAME)

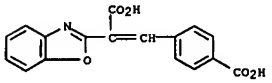


RN 142885-78-7 CAPLUS
CN 1H-Benzimidazole-2-acetic acid, α-[(3-bromo-4-methoxyphenyl)methylene]-5-methoxy- (9CI) (CA INDEX NAME)

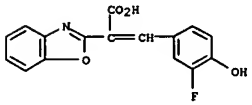


RN 142885-79-8 CAPLUS
CN 2-Benzoxazoleacetic acid, α-[(3-fluoro-4-hydroxyphenyl)methylene]-

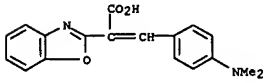
L4 ANSWER 138 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



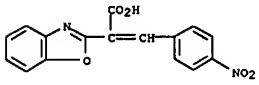
L4 ANSWER 138 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



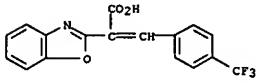
RN 142885-80-1 CAPLUS
CN 2-Benzoxazoleacetic acid, α-[[4-(dimethylamino)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 142885-81-2 CAPLUS
CN 2-Benzoxazoleacetic acid, α-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)



RN 142885-82-3 CAPLUS
CN 2-Benzoxazoleacetic acid, α-[[4-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 142885-83-4 CAPLUS
CN 2-Benzoxazoleacetic acid, α-[(4-carboxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 139 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

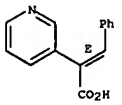
ACCESSION NUMBER: 1992:255088 CAPLUS
DOCUMENT NUMBER: 116:255088
TITLE: Substituent effects on the carbon-13 chemical shifts in α-phenylpyridylacrylic acids
AUTHOR(S): Jovanovic, B. Z.; Misic-Vukovic, M.; Vajs, V. E.; Canadi, J. J.
CORPORATE SOURCE: Fac. Technol. Metall., Univ. Belgrade, Belgrade, 11001, Yugoslavia
SOURCE: Journal of Molecular Structure (1992), 267, 411-14
CODEN: JMOSB4; ISSN: 0022-2860
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The 13C NMR spectra of some substituted α-phenylpyridylacrylic acids, α-Ph-, α-(3-pyrydyl)- and α-(3-pyrydyl N-oxide)cinnamic acids were determined in DMSO-d6. The substituent chemical shifts for Cβ atom ethylenic bond of the examined compds. correlated linearly with the sum of the corresponding substituent consts. in the both rings. This correlation was interpreted as evidence that the electronic effects of both substituents are involved in conjugated aromatic system.

IT 141694-17-9 141694-18-0
RL: PRP (Properties)
(carbon-13 NMR of)

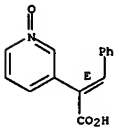
RN 141694-17-9 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 141694-18-0 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, 1-oxide, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 140 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

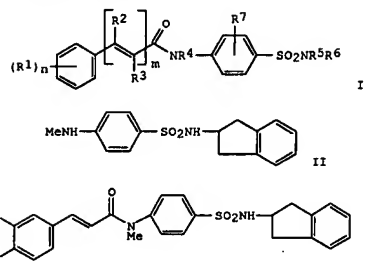
ACCESSION NUMBER: 1992:128365 CAPLUS
DOCUMENT NUMBER: 116:128365
TITLE: Preparation of benzenesulfonamides as phospholipase A2 inhibitors
INVENTOR(S): Oinuma, Hitoshi; Hasegawa, Takashi; Takamura, Tadanobu; Nomoto, Kenichi; Daiku, Yoshiharu; Naito, Toshihiko; Hamano, Sachiyuki
PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan
SOURCE: PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9112237	A1	19910822	WO 1991-JP149	19910207
W: CA, FI, JP, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
CA 2050591	A1	19910809	CA 1991-2050591	19910207
EP 468054	A1	19920129	EP 1991-903288	19910207
EP 468054	B1	19970528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 153655	T	19970615	AT 1991-903288	19910207
ES 2100943	T3	19970701	ES 1991-903288	19910207
JP 3176365	B2	20010618	JP 1991-503825	19910207
US 5281626	A	19940125	US 1991-768515	19910926
NO 9103829	A	19911206	NO 1991-3829	19910930
US 5530118	A	19960625	US 1993-161817	19931206
US 5663414	A	19970902	US 1995-581257	19951229

PRIORITY APPLN. INFO.: JP 1990-27071 A 19900208
JP 1991-27071 A 19910207
WO 1991-JP149 W 19910207
US 1991-768515 A3 19910926
US 1993-161817 A3 19931206

OTHER SOURCE(S): MARPAT 116:128365
GI

L4 ANSWER 140 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

II

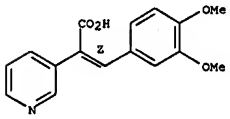
III

AB The title compds. [I; R1 = H, cyano, NO2, OH, etc.; R2 = H, pyridyl; R3 = H, alkyl, cyano, etc.; R4 = H, alkyl; R5, R6 = H, (hydroxy)alkyl, (di)(alkyl)amino, R5R6N = heterocyclyl, etc.; R7 = H, alkyl, alkoxy; m = 1, 2; n = 1-4], useful in preventing and treating ischemia, myocardial infarction, angina pectoris, etc., are prepared A solution of 3,4-diacetoxycinnamoyl chloride in CH2Cl2 was added dropwise to a solution of sulfonamide II (preparation given) in pyridine at 0° and the solution was stirred at room temperature to give 100% diamide III (R = Ac), which was hydrolyzed with concentrated HCl in MeOH-THF at 60° to give 93% III (R = H). The latter inhibited phospholipase A2 with IC30 of 4.48 μM, vs. >100 μM with mepacrine. Also prepared and tested were 97 addnl. I.

IT 137473-33-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of phospholipase A2 inhibitor)

RN 137473-33-7 CAPLUS
CN 3-Pyridineacetic acid, α-[(3,4-dimethoxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



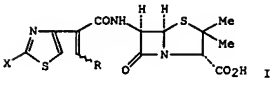
L4 ANSWER 141 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:679691 CAPLUS
DOCUMENT NUMBER: 115:279691
TITLE: Preparation of 6β-[2-(2-aminothiazol-4-yl)acrylamido]penicillanates
INVENTOR(S): Ponsford, Roger John; Stachulski, Andrew Valentine
PATENT ASSIGNEE(S): Beecham Group PLC, UK
SOURCE: Eur. Pat. Appl., 33 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 421752	A2	19910410	EP 1990-310810	19901003
EP 421752	A3	19920122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03271292	A	19911203	JP 1990-68504	19900320
CA 2026786	A1	19910406	CA 1990-2026786	19901003
AU 9063780	A	19910411	AU 1990-63780	19901003
HU 55789	A2	19910628	HU 1990-6325	19901003
ZA 9007896	A	19920129	ZA 1990-7896	19901003
NO 9004319	A	19910408	NO 1990-4319	19901004
CN 1051562	A	19910522	CN 1990-108848	19901005
JP 03151389	A	19910627	JP 1990-268244	19901005

PRIORITY APPLN. INFO.: GB 1989-22411 A 19891005
GB 1990-16896 A 19900801

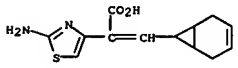
OTHER SOURCE(S): MARPAT 115:279691
GI



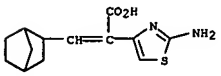
I

AB Title compds. [I; X = H, NHR1; R1 = H, protecting group; R = (substituted) (heteroatom-containing) bicyclyl] and salts and esters thereof, were prepared as antibacterials (no data). Thus, 2-norbornanemethanol (preparation given), Me 2-acetamidothiazol-4-acetate, piperidine, and HOAc were refluxed 25 h in PhMe with a water separator to give Me E,Z-[2-(2-acetamidothiazol-4-yl)-3-(bicyclo[2.2.1]hept-2-yl)]propenoate as a separable mixture The Z-isomer was saponified with 1M NaOH/dioxane and the free acid was converted to the active ester with DCC in DMF. The ester was added to 6-aminopenicillanic acid in 1M NaOH followed by stirring for 2.5 h to give Z-I [X = H2N, R = bicyclo[2.2.1]hept-2-yl] Na salt. I are said to be broad-spectrum antibacterials with high stability to β-lactamase.

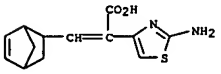
L4 ANSWER 141 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 135577-02-5P 135577-08-1P 135577-09-2P
135577-12-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 135577-02-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[4.1.0]hept-3-en-7-ylmethylene)-, [1α,6α,7β(Z)]- (9CI) (CA INDEX NAME)



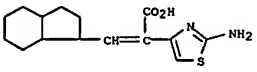
RN 135577-08-1 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.1]hept-2-ylmethylene)-, [1α,2β(Z),4α]- (9CI) (CA INDEX NAME)



RN 135577-09-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.1]hept-5-en-2-ylmethylene)-, [1α,2β(Z),4α]- (9CI) (CA INDEX NAME)

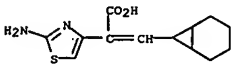


RN 135577-12-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(octahydro-1H-inden-1-yl)methylene]-, [1α(Z),3aβ,7aβ]- (9CI) (CA INDEX NAME)

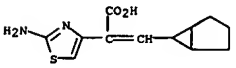


IT 135577-29-6P 135577-31-0P 135577-35-4P
135577-38-7P 135577-39-8P 135577-43-4P
135577-46-7P 135577-49-0P 135577-52-5P

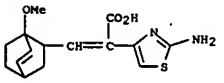
L4 ANSWER 141 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



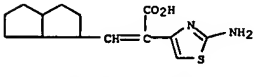
RN 135577-39-8 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[3.1.0]hex-6-ylmethylene)-, [1α,5α,6α(Z)]- (9CI) (CA INDEX NAME)



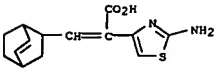
RN 135577-43-4 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(1-methoxybicyclo[2.2.2]oct-5-en-2-yl)methylene]-, [1α,2β(Z),4β]- (9CI) (CA INDEX NAME)



RN 135577-46-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(octahydro-1-pentalenyl)methylene]- (9CI) (CA INDEX NAME)

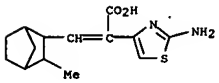


RN 135577-49-0 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.2]oct-5-en-2-ylmethylene)-, [1α,2α(Z),4α]- (9CI) (CA INDEX NAME)

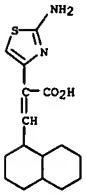


RN 135577-52-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[5.1.0]oct-8-ylmethylene)-,

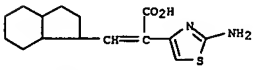
L4 ANSWER 141 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
135637-88-6P 135637-89-7P 135637-96-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for acrylamidopenicillanate)
RN 135577-29-6 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(3-methylbicyclo[2.2.1]hept-2-yl)methylene]- (9CI) (CA INDEX NAME)



RN 135577-31-0 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(decahydro-1-naphthalenyl)methylene]- (9CI) (CA INDEX NAME)

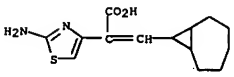


RN 135577-35-4 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(octahydro-1H-inden-1-yl)methylene]-, [1α(Z),3aα,7aα]- (9CI) (CA INDEX NAME)

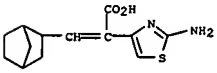


RN 135577-38-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[4.1.0]hept-7-ylmethylene)-, [1α,6α,7α(Z)]- (9CI) (CA INDEX NAME)

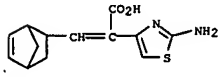
L4 ANSWER 141 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
[1α,7α,8α(Z)]- (9CI) (CA INDEX NAME)



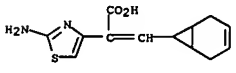
RN 135637-88-6 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.1]hept-2-ylmethylene)-, [1α,2α(Z),4α]- (9CI) (CA INDEX NAME)



RN 135637-89-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[2.2.1]hept-5-en-2-ylmethylene)-, [1α,2α(Z),4α]- (9CI) (CA INDEX NAME)

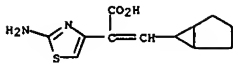


RN 135637-96-6 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[4.1.0]hept-3-en-7-ylmethylene)-, [1α,6α,7α(Z)]- (9CI) (CA INDEX NAME)



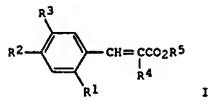
IT 135638-06-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for acrylamidopenicillanate antibacterial)
RN 135638-06-1 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(bicyclo[3.1.0]hex-6-ylmethylene)-, [1α,5α,6β(Z)]- (9CI) (CA INDEX NAME)

L4 ANSWER 141 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 142 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:135564 CAPLUS
DOCUMENT NUMBER: 114:135564
TITLE: Anti-anoxia effect of 33 compounds derived from phenylacrylic acid in mice
AUTHOR(S): Dai, Dezai; Li, Qiheng; Ma, Erli; Wang, Zhennan
CORPORATE SOURCE: Div. Pharmacol., China Pharm. Univ., Nanjing, Peop. Rep. China
SOURCE: Zhongguo Yaoke Daxue Xuebao (1990), 21(3), 170-2
CODEN: ZHYXE9; ISSN: 1000-5048
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

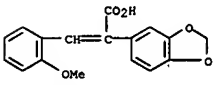


I

AB Compds. derived from phenylacrylic acid (I; R1 = H, OMe, CN, or Br; R2 = R3 = H, OH, OMe, or CH2O2; R4 = H or others; and R5 = H, Me, Et, or Pr) possess anti-anoxia activity if a OH group is selectively located at m-position of the Ph ring as tested in mice. However, no anti-anoxia effect will be observed if another OH group is attached to p-position. Other compds. are active with the following substituents: a MeO group on the Ph ring or an aromatic ring attached to the a-position of the side chain.

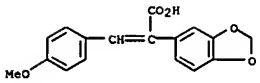
IT 87751-89-1 87751-90-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antianoxic activity of, structure in relation to)

RN 87751-89-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 87751-90-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 142 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 143 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

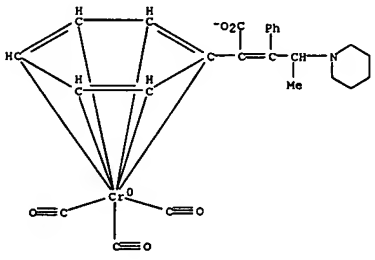
ACCESSION NUMBER: 1991:43041 CAPLUS
DOCUMENT NUMBER: 114:43041
TITLE: A new reaction of aminocarbene complexes of chromium upon alkyne insertions: deoxygenation rearrangement of ketene intermediates. Formation and x-ray structure of a tetrahydroindolizine complex
AUTHOR(S): Denise, B.; Goumont, R.; Parlier, A.; Rudler, H.; Daran, J. C.; Vaissermann, J.
CORPORATE SOURCE: Lab. Chim. Org., Univ. Pierre et Marie Curie, Paris, 75252, Fr.
SOURCE: Journal of the Chemical Society, Chemical Communications (1990), (18), 1238-40
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:43041
GI For diagram(s), see printed CA Issue.

AB Aminocarbene complexes I [R = H, Me; n = 4, 5, 7) react with PhC.tplbond.CPh to give besides the expected heterocyclic compds. originating from cascade alkyne-CO insertion-rearrangement reactions, deoxygenation-rearrangement products II of ketene intermediates, whereas when the nitrogen bears substituents of low migratory aptitude, ketene complexes III and their derivs. IV could be isolated. The crystal structures of II (R = Me, n = 4) and IV (R = H, n = 5) were determined

IT 131374-61-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 131374-61-3 CAPLUS
CN Chromate(1-), tricarbonyl[(1,2,3,4,5,6-η)-α-[(1E)-1-phenyl-2-(1-piperidinyl)propylidene]benzeneacetato]-, hydrogen (9CI) (CA INDEX NAME)

PAGE 1-A

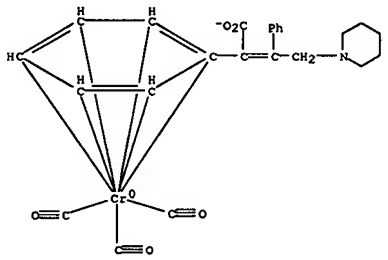


PAGE 2-A

● H+

L4 ANSWER 143 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 131374-63-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal and mol. structure of)
RN 131374-63-5 CAPLUS
CN Chromate(1-), tricarbonyl[(1,2,3,4,5,6-η)-α-[(1E)-1-phenyl-2-(1-piperidinyl)ethylidene]benzeneacetato]-, hydrogen (9CI) (CA INDEX NAME)

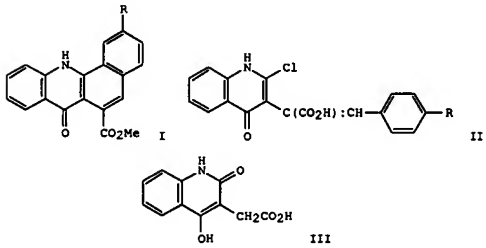
PAGE 1-A



PAGE 2-A

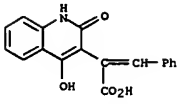
● H+

L4 ANSWER 144 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:42536 CAPLUS
DOCUMENT NUMBER: 114:42536
TITLE: A new facile synthesis of benz[c]acridines
AUTHOR(S): Jayabalan, L.; Shanmugam, P.
CORPORATE SOURCE: Dep. Chem., Bharathiar Univ., Coimbatore, 641 046, India
SOURCE: Synthesis (1990), (9), 789-94
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:42536
GI

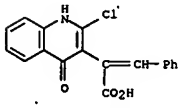


AB A photochem. synthesis of benzacridines (I; R = H, Cl, OMe) using chloro(carboxyphenylethenyl)quinolinones (II) as precursors is reported. The precursor quinolinones (II) are obtained from hydroxyquinolinoneacetic acid (III).
IT 131469-31-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and lactonization of)
RN 131469-31-3 CAPLUS
CN 3-Quinolineacetic acid, 1,2-dihydro-4-hydroxy-2-oxo-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

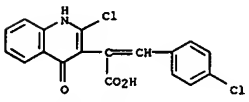
L4 ANSWER 144 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



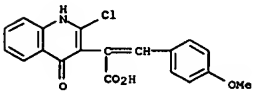
IT 131469-38-0P 131469-39-1P 131469-40-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and/or tautomer, methylation and photocyclization of)
RN 131469-38-0 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-1,4-dihydro-4-oxo-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 131469-39-1 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-α-[(4-chlorophenyl)methylene]-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

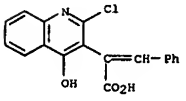


RN 131469-40-4 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-1,4-dihydro-α-[(4-methoxyphenyl)methylene]-4-oxo- (9CI) (CA INDEX NAME)

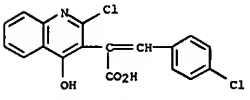


IT 131469-55-1P 131469-56-2P 131469-57-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and/or tautomer, methylation, and photocyclization of)

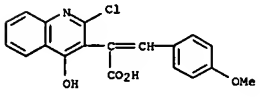
L4 ANSWER 144 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 131469-55-1 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-4-hydroxy-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 131469-56-2 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-α-[(4-chlorophenyl)methylene]-4-hydroxy- (9CI) (CA INDEX NAME)



RN 131469-57-3 CAPLUS
CN 3-Quinolineacetic acid, 2-chloro-4-hydroxy-α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 145 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:611987 CAPLUS
DOCUMENT NUMBER: 113:211987
TITLE: Preparation of tetrazolyldiarylalkenoates as hypocholesteremics
INVENTOR(S): Sit, Sing Yuen; Wright, John J.
PATENT ASSIGNEE(S): Bristol-Myers Co., USA
SOURCE: U.S., 69 pp. Cont.-in-part of U.S. Ser. No. 18,542.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4897490	A	19900130	US 1988-151513	19880218
DK 8800972	A	19880826	DK 1988-972	19880224
DK 174822	B1	20031208		
FI 8800869	A	19880826	FI 1988-869	19880224
FI 96601	B	19960415		
FI 96601	C	19960725		
NO 8800809	A	19880826	NO 1988-809	19880224
NO 169438	B	19920316		
NO 169438	C	19920624		
WO 8806584	A1	19880907	WO 1988-US462	19880224
W: AU, DK, FI, HU, JP, KR, NO				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DE 3805801	A1	19880908	DE 1988-3805801	19880224
DE 3805801	C2	20010301		
NL 8800465	A	19880916	NL 1988-465	19880224
SE 8800638	A	19880921	SE 1988-638	19880224
SE 503618	C2	19960715		
AU 8813950	A	19880926	AU 1988-13950	19880224
FR 2612924	A1	19880930	FR 1988-2211	19880224
FR 2612924	B1	19910111		
ZA 8801279	A	19890222	ZA 1988-1279	19880224
HU 47259	A2	19890228	HU 1988-886	19880224
HU 204038	B	19911128		
JP 01502269	T	19890810	JP 1988-502491	19880224
ES 2010246	A6	19891101	ES 1988-532	19880224
CS 271481	B2	19901012	CS 1988-1180	19880224
CH 676848	A5	19910315	CH 1988-692	19880224
HU 203329	B	19910729	HU 1990-669	19880224
HU 204516	B	19920128	HU 1989-6737	19880224
AT 8800461	A	19920615	AT 1988-461	19880224
AT 395589	B	19930125		
IL 85529	A	19930131	IL 1988-85529	19880224
IL 101849	A	19930315	IL 1988-101849	19880224
CA 1328268	C	19940405	CA 1988-559667	19880224
AU 8812172	A	19880901	AU 1988-12172	19880225
AU 601264	B2	19900906		
CN 88100911	A	19880928	CN 1988-100911	19880225
CN 1026110	B	19941005		
GB 2202846	A	19881005	GB 1988-4473	19880225
GB 2202846	B	19910515		

L4 ANSWER 145 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

DD 279880	A5	19900620	DD 1988-313201	19880225
BE 1002116	A3	19900710	BE 1988-220	19880225
ES 2026746	A6	19920501	ES 1989-2217	19890623
US 5068346	A	19911126	US 1989-437942	19891117
US 5110940	A	19920505	US 1991-695827	19910506
NO 9103089	A	19880826	NO 1991-3089	19910808
AT 9200382	A	19951115	AT 1992-382	19920228
AT 401175	B	19960725		
AT 9200379	A	19960215	AT 1992-379	19920228
AT 401518	B	19960925		
FI 9502243	A	19950509	FI 1995-2243	19950509
FI 103793	B	19990930		
FI 103793	B1	19990930		

PRIORITY APPLN. INFO.:

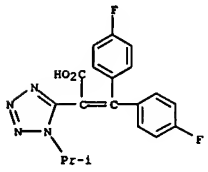
US 1987-18542	A2	19870225
US 1988-151513	A	19880218
AT 1988-461	A	19880224
FI 1988-869	A	19880224
GB 1988-4235	A	19880224
IL 1988-85529	A3	19880224
NO 1988-809	A1	19880224
WO 1988-US462	A	19880224
US 1989-437942	A3	19891117

OTHER SOURCE(S): CASREACT 113:211987; MARPAT 113:211987
GI

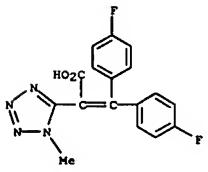
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. (I; A = Q3, Q4; R1,R4 = H, halo, alkyl, alkoxy, CF3; R2,R3,R5,R6 = H, halo, alkyl, alkoxy; T = Q1, Q2; R7 = H, alkyl, alkoxyalkyl, CH2OCH2CH2OMe; R8 = H, hydrolyzable ester group, cation; X = OH, O) were prepared Thus, (2,4-FMeC6H3)2CO (preparation given) was condensed with 1,5-dimethyltetrazole and the product converted in 2 steps to R2C:CT(CH:CH)nA (R = 2,4-FMeC6H3, T = 1-methyl-1H-tetrazol-5-yl) (II; A = CHO, n = 0) which was condensed with PH3P:CHCHO to give II (A = CHO, n = 1). The latter underwent aldol condensation with MeCOCH2CO2CMe3 to give, after reduction and saponification, title compound III which had IC50 of 0.029 μM for inhibition of microsomal HMG-CoA reductase in vitro.
IT 118845-64-0P 118875-13-1P 118875-14-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for hypocholesteremic)
RN 118845-64-0 CAPLUS

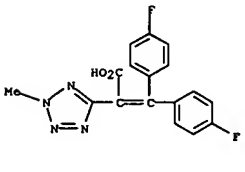
L4 ANSWER 145 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-1-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 118875-13-1 CAPLUS
CN 1H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-1-methyl- (9CI) (CA INDEX NAME)



RN 118875-14-2 CAPLUS
CN 2H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-2-methyl- (9CI) (CA INDEX NAME)



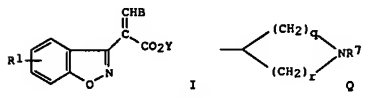
L4 ANSWER 146 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:532165 CAPLUS
DOCUMENT NUMBER: 113:132165
TITLE: Preparation of benzisoxazolylacrylic acid derivatives as antispasmodics
INVENTOR(S): Naruto, Shunsuke; Nagamoto, Norio; Kadokawa, Toshiaki; Kawashima, Katsuyoshi
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02083374	A	19900323	JP 1988-237814	19880921

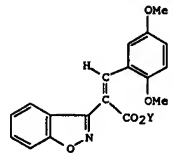
PRIORITY APPLN. INFO.:

JP 1988-237814	19880921

OTHER SOURCE(S): MARPAT 113:132165
GI



I

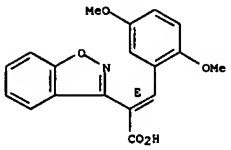


II

AB The title compds. [I; R1 = H, halo, alkoxy; B = (substituted) Ph, 1-naphthyl, thienyl, furyl; Y = (CH2)mCHR4(CH2)nNR5R6, Q wherein R4 = H, alkyl; R5, R6 = alkyl, R5R6N = saturated heterocyclyl; R7 = alkyl, 1,3-dioxolan-4-ylmethyl; m, n = 0-3; m + n = 1-4; q, r = 1-3, q + r = 3-5], useful as acetylcholine antagonists and antispasmodics, are prepared Refluxing 1.0 g acid II (Y = H) with SOCl2 in MePh gave the acid chloride, which was heated with 1 g Et2N(CH2)3OH and 1.5 mL Et3N in MePh at 100° to give 1.1 g (E)-II.HBr [Y = Et2N(CH2)3] (III) after treatment with HBr. III showed antispasmodic activity with ID50 of 6.0 + 10-7 g/mL in guinea pigs. Among 71 addnl. I prepared, 28 showed antispasmodic activity.
IT 129142-26-3P 129142-27-4P 129142-28-5P

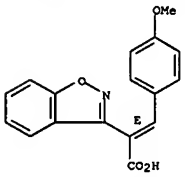
L4 ANSWER 146 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
129142-30-9P 129142-31-0P 129142-32-1P
129142-33-2P 129142-34-3P 129142-35-4P
129142-36-5P 129142-37-6P 129142-38-7P
129142-39-8P 129142-40-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and esterification of)
RN 129142-26-3 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(2,5-dimethoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 129142-27-4 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(4-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

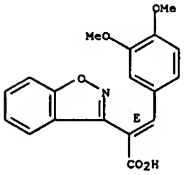
Double bond geometry as shown.



RN 129142-28-5 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(2,5-dimethoxyphenyl)methylene]-5-methoxy-, (E)- (9CI) (CA INDEX NAME)

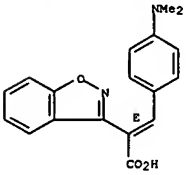
Double bond geometry as shown.

L4 ANSWER 146 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



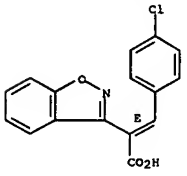
RN 129142-33-2 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[[4-(dimethylamino)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



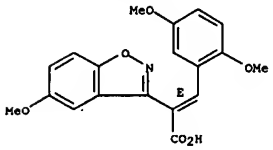
RN 129142-34-3 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(4-chlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



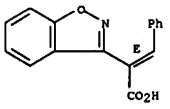
RN 129142-35-4 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(4-nitrophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

L4 ANSWER 146 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



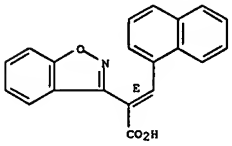
RN 129142-30-9 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 129142-31-0 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-(1-naphthalenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

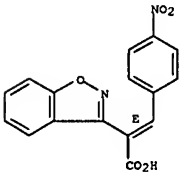
Double bond geometry as shown.



RN 129142-32-1 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(3,4-dimethoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

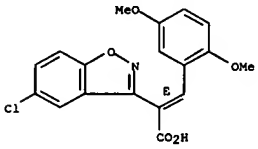
Double bond geometry as shown.

L4 ANSWER 146 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



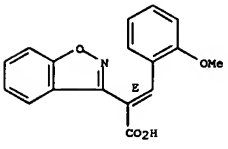
RN 129142-36-5 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, 5-chloro-α-[(2,5-dimethoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 129142-37-6 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(2-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

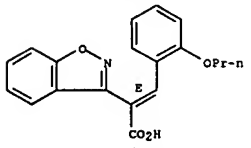
Double bond geometry as shown.



RN 129142-38-7 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(2-propoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

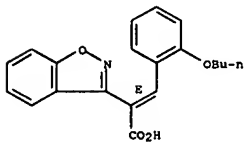
Double bond geometry as shown.

L4 ANSWER 146 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



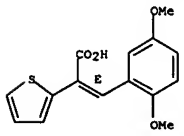
RN 129142-39-8 CAPLUS
CN 1,2-Benzisoxazole-3-acetic acid, α-[(2-butoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 129142-40-1 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2,5-dimethoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 147 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

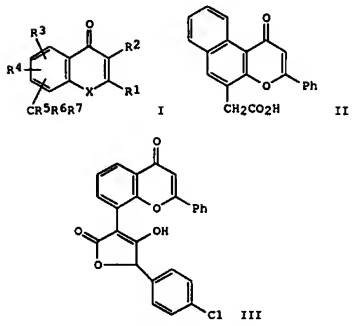
ACCESSION NUMBER: 1990:423516 CAPLUS
DOCUMENT NUMBER: 113:23516
TITLE: Flavonoid compounds as anticancer agents and immunostimulants and their preparation
INVENTOR(S): Briet, Philippe; Berthelon, Jean Jacques; Collonges, Francois
PATENT ASSIGNEE(S): LIPHA, Lyonnaise Industrielle Pharmaceutique, Fr.
SOURCE: Eur. Pat. Appl., 106 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 341104	A2	19891108	EP 1989-400953	19890406
EP 341104	A3	19891129		
EP 341104	B1	19931229		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
IL 89840	A	19961031	IL 1989-89840	19890404
NO 8901415	A	19891009	NO 1989-1415	19890405
NO 172344	B	19930329		
NO 172344	C	19930707		
ZA 8902523	A	19900530	ZA 1989-2523	19890405
SU 1739846	A3	19920607	SU 1989-4613889	19890405
CA 1325205	C	19931214	CA 1989-595750	19890405
DK 8901667	A	19891007	DK 1989-1667	19890406
AU 8932505	A	19891012	AU 1989-32505	19890406
AU 630345	B2	19921029		
HU 49600	A2	19891030	HU 1989-1658	19890406
HU 206701	B	19921228		
JP 02006473	A	19900110	JP 1989-87838	19890406
DD 283816	A5	19901024	DD 1989-327362	19890406
AT 99302	T	19940115	AT 1989-400953	19890406
ES 2060799	T3	19941201	ES 1989-400953	19890406
IN 170909	A1	19920613	IN 1989-DE480	19890531
US 5116954	A	19920526	US 1989-388738	19890802
US 1427	H	19950404	US 1992-892706	19920529

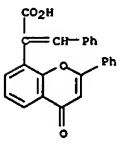
PRIORITY APPLN. INFO.: US 1988-178315 A 19880406
US 1988-233423 B1 19880818
EP 1989-400953 A 19890406

OTHER SOURCE(S): MARPAT 113:23516
GI

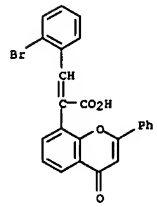
L4 ANSWER 147 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. I [X = N (sic), O, Se, etc.; R1 = H, C1-7 alkyl, naphthyl, (substituted) Ph, etc.; R2 = H, Ph, OH, C1-3 alkyl, alkoxy; R3, R4 = H, C1-6 alkyl, OH, C1-6 alkoxy, halo; R5 = H, C1-3 alkyl, CN, etc.; R6 = H, C1-6 alkyl, OH, etc.; or CR5R6 = C:NOH, C:O, etc.; R7 = CO(C1-6 alkyl), S(C1-6 alkyl), SH, SCO(C1-3 alkyl), etc.] are prepared A mixture of 1-oxo-3-phenyl-1H-naphtho[2,1-b]pyran-5-acetonitrile, AcOH, H2O, and H2SO4 was refluxed to give naphthopyranacetic acid II. Benzopyran III at 1000 μg per disk exhibited an inhibition value of 400 against the PO3 tumor.
IT 127768-67-6P 127768-68-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as anticancer agent)
RN 127768-67-6 CAPLUS
CN 4H-1-Benzopyran-8-acetic acid, 4-oxo-2-phenyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



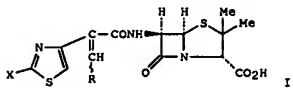
L4 ANSWER 147 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 127768-68-7 CAPLUS
CN 4H-1-Benzopyran-8-acetic acid, α-[(2-bromophenyl)methylene]-4-oxo-2-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 148 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:216542 CAPLUS
DOCUMENT NUMBER: 112:216542
TITLE: 6-Substituted acrylamidopenicillanic acid derivatives,
preparation and use
INVENTOR(S): Ponsford, Roger John; Stachulski, Andrew Valentine
PATENT ASSIGNEE(S): Beecham Group PLC, UK
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 337643	A2	19891018	EP 1989-303318	19890404
EP 337643	A3	19910508		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8901619	A	19891007	DK 1989-1619	19890404
NO 8901403	A	19891009	NO 1989-1403	19890404
AU 8932424	A	19891012	AU 1989-32424	19890404
AU 617783	B2	19911205		
ZA 8902463	A	19910130	ZA 1989-2463	19890404
FI 8901640	A	19891007	FI 1989-1640	19890405
JP 01305093	A	19891208	JP 1989-86696	19890405
US 4954489	A	19900904	US 1989-333554	19890405
HU 50186	A2	19891228	HU 1989-1663	19890406
PRIORITY APPLN. INFO.:			GB 1988-8032 A	19880406
			GB 1988-18513 A	19880804
			GB 1988-22511 A	19880926

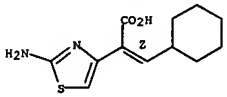
OTHER SOURCE(S): MARPAT 112:216542
GI



AB The title compds. I [X = H, NHR1; R1 = H, amino protecting group; R = (substituted) cycloalkyl, cycloalkenyl], pharmaceutically acceptable salts, and in vivo hydrolyzable esters thereof are prepared as antibiotics.
Na 6β-[(Z)-2-(2-aminothiazol-4-yl)-3-cyclohexyl]propenamidopenicillanate [prepared from (Z)-[2-(2-aminothiazol-4-yl)-3-cyclohexyl]propenoic acid
and 6-aminopenicillanic acid] in vitro exhibited a min. inhibitory concentration

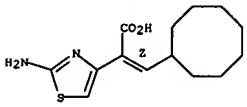
L4 ANSWER 148 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
of 0.12 μg against Escherichia coli 10418.
IT 126781-75-7P 126781-80-4P 126781-81-5P
126781-84-8P 126781-88-2P 126781-90-6P
126781-95-1P 126781-99-5P 126782-01-2P
126782-05-6P 126782-06-7P 126873-34-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antibiotic)
RN 126781-75-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(cyclohexylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



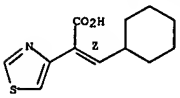
RN 126781-80-4 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(cyclooctylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



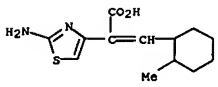
RN 126781-81-5 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclohexylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

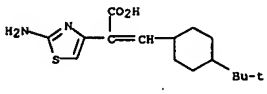


RN 126781-84-8 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(2-methylcyclohexyl)methylene]-

L4 ANSWER 148 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

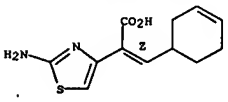


RN 126781-88-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[[4-(1,1-dimethylethyl)cyclohexyl]methylene]-, [1α(Z),4β]- (9CI) (CA INDEX NAME)

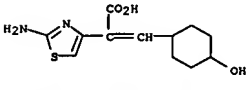


RN 126781-90-6 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(3-cyclohexen-1-ylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



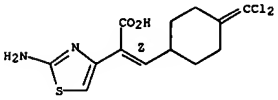
RN 126781-95-1 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(4-hydroxycyclohexyl)methylene]-, [1α(Z),4β]- (9CI) (CA INDEX NAME)



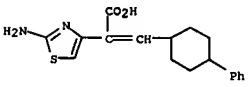
RN 126781-99-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[[4-(dichloromethylene)cyclohexyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 148 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

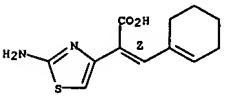


RN 126782-01-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(4-phenylcyclohexyl)methylene]-, [1α(Z),4α]- (9CI) (CA INDEX NAME)



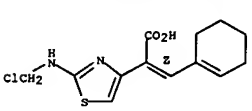
RN 126782-05-6 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(1-cyclohexen-1-ylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



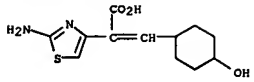
RN 126782-06-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-[(chloromethyl)amino]-α-(1-cyclohexen-1-ylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 126873-34-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(4-hydroxycyclohexyl)methylene]-, [1α(Z),4α]- (9CI) (CA INDEX NAME)

L4 ANSWER 148 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

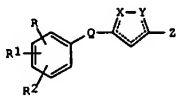


L4 ANSWER 149 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

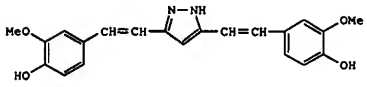
ACCESSION NUMBER: 1990:178969 CAPLUS
DOCUMENT NUMBER: 112:178969
TITLE: Preparation of styrylpyrazoles, styrylisoxazoles, and analogs as inhibitors of 5-lipoxygenase and cyclooxygenase and as sunscreens
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: Austrian, 45 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 389106	B	19891025	AT 1987-2649	19871008
AT 8702649	A	19890315		
PRIORITY APPLN. INFO.:			AT 1987-2649	19871008

OTHER SOURCE(S): CASREACT 112:178969; MARPAT 112:178969
GI



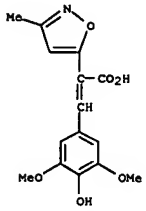
I



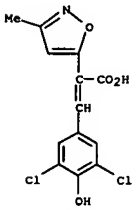
II

AB Title compds. I [R, R1, R2 = H, alkyl, OH, OR3, CO2R4, OCOR3, COR3, NR6R7, NHCOR3, NHCHO, NHSO2R3, NHCONHR4, CH2OH, halo, CF3, SR4, NO2; R3 = alkyl; R4, R6-R9 = H, alkyl; X, Y = N, NR5, O, S; R5 = H, alkyl, CHR8CO2R9, COR4, cycloalkyl, aryl, aralkyl; Q = (CH2)n, CH:CH, CH:C(CO2R4); n = 0-4; Z = H, alkyl, aryl, aralkyl, OCOR3, CO2R4, COR3, CHR8CO2R9, halo, CF3, CH:CHC6H3RR1R2, heteroaryl, heteroaralkyl; with various provisos, especially on X and Y], were prepared Thus, cyclocondensation of curcumin, i.e. 1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, with N2H4 in EtOH/BuOH containing AcOH at 60° gave bis[(hydroxymethoxyphenyl)ethenyl]pyrazole II. The IC50 of II for inhibition of 5-lipoxygenase in vitro was 1.0 μM.
IT 113465-45-5P 113465-46-6P 113465-47-7P

L4 ANSWER 149 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
113465-48-8P 113465-49-9P 113465-50-2P
113465-51-3P 113465-52-4P 113465-60-4P
113465-61-5P 113465-62-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as lipoxygenase inhibitor)
RN 113465-45-5 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3,5-dimethoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

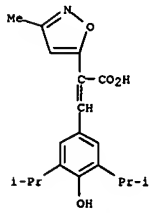


RN 113465-46-6 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(3,5-dichloro-4-hydroxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

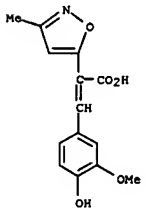


RN 113465-47-7 CAPLUS
CN 5-Isoxazoleacetic acid, α-[[4-hydroxy-3,5-bis(1-methylethyl)phenyl]methylene]-3-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 149 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

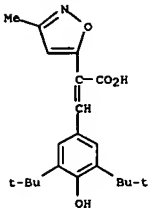


RN 113465-48-8 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3-methoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

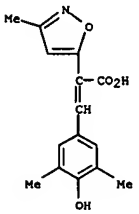


RN 113465-49-9 CAPLUS
CN 5-Isoxazoleacetic acid, α-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]-3-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 149 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

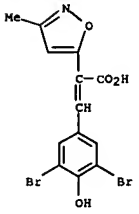


RN 113465-50-2 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3,5-dimethylphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

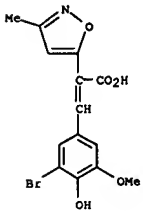


RN 113465-51-3 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(3,5-dibromo-4-hydroxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

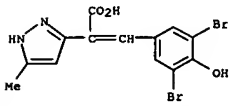
L4 ANSWER 149 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 113465-52-4 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(3-bromo-4-hydroxy-5-methoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

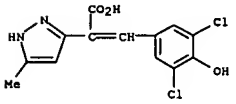


RN 113465-60-4 CAPLUS
CN 1H-Pyrazole-3-acetic acid, α-[(3,5-dibromo-4-hydroxyphenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)

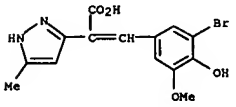


RN 113465-61-5 CAPLUS

L4 ANSWER 149 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Pyrazole-3-acetic acid, α-[(3,5-dichloro-4-hydroxyphenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)



RN 113465-62-6 CAPLUS
CN 1H-Pyrazole-3-acetic acid, α-[(3-bromo-4-hydroxy-5-methoxyphenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)

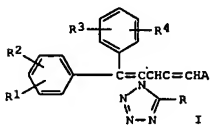


L4 ANSWER 150 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1990:139037 CAPLUS
DOCUMENT NUMBER:	112:139037
TITLE:	Preparation of antihypercholesterolemic tetrazol-1-yl compounds
INVENTOR(S):	Sit, Sing Yuen; Wright, John J.
PATENT ASSIGNEE(S):	Bristol-Myers Co., USA
SOURCE:	U.S., 21 pp. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4870187	A	19890926	US 1988-235355	19880823
US 5010205	A	19910423	US 1989-386373	19890728
EP 355820	A1	19900228	EP 1989-115589	19890823
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 02073074	A	19900313	JP 1989-215141	19890823
US 5070206	A	19911203	US 1991-654698	19910213
PRIORITY APPLN. INFO.:			US 1988-235355	A3 19880823
			US 1989-386373	A3 19890728

OTHER SOURCE(S): CASREACT 112:139037; MARPAT 112:139037
GI

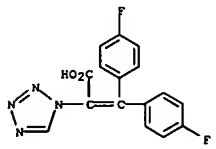


AB Title compds. I (R = H, C1-4 alkyl, Ph; R1-R4 = H, halo, C1-4 alkyl, C1-4 alkoxy, F3C; A = CH(OH)CH2CH(OH)CH2CO2R5, tetrahydro-4-hydroxy-2-oxo-2H-pyranyl; R5 = H, hydrolyzable ester, cation) pharmaceutically acceptable salt, are prepared I are also useful in treatment of hyperlipoproteinemia, and atherosclerosis. Intermediates for preparation of I are also prepared I (R, R1, R3 = H; R2, R4 = F; A = CH(OH)CH2CH(OH)CO2R5, R5 = Et) (preparation given) in THF under Ar was saponified with aqueous NaOH to give I (R5 = H).Na salt (II). The antihypercholesterolemic activity of II was demonstrated by in vitro inhibition of 3-hydroxy-3-methylglutaryl CoA reductase (IC50 0.12 μM).

IT 125485-59-8
RL: PROC (Process)
(conversion of, to alc.)

RN 125485-59-8 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[bis(4-fluorophenyl)methylene]- (9CI)

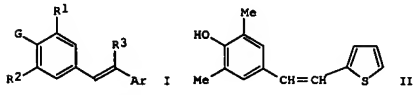
L4 ANSWER 150 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)



L4 ANSWER 151 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:118636 CAPLUS
DOCUMENT NUMBER: 112:118636
TITLE: Arylethenylphenol (and especially thienylethenylphenol) derivatives useful as inhibitors of 5-lipoxygenase, and their preparation and pharmaceutical compositions
INVENTOR(S): Lazer, Edward S.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

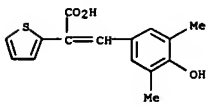
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 334119	A1	19890927	EP 1989-104251	19890310
EP 334119	B1	19930616		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 90674	T	19930715	AT 1989-104251	19890310
ES 2056983	T3	19941016	ES 1989-104251	19890310
NO 8901114	A	19890922	NO 1989-1114	19890315
NO 169648	B	19920413		
NO 169648	C	19920722		
AU 8931514	A	19890921	AU 1989-31514	19890320
AU 628324	B2	19920917		
DK 8901344	A	19890922	DK 1989-1344	19890320
FI 8901295	A	19890922	FI 1989-1295	19890320
HU 50093	A2	19891228	HU 1989-1323	19890320
HU 207858	B	19930628		
JP 02004729	A	19900109	JP 1989-69109	19890320
DD 283602	A5	19901017	DD 1989-326756	19890320
ZA 8902086	A	19901128	ZA 1989-2086	19890320
PRIORITY APPLN. INFO.:			US 1988-170512 A	19880321
			EP 1989-104251 A	19890310

OTHER SOURCE(S): MARPAT 112:118636
GI

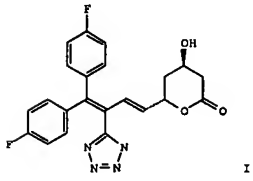


AB Title compds. I [R1, R2 = alkyl, allyl, alkoxy, halo; R3 = H, alkyl, CO2H,

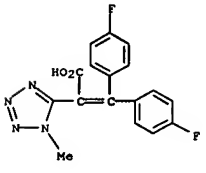
L4 ANSWER 151 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
alkoxycarbonyl; G = OH, OCOXCO2H, OCO(CHR4)nNR5R6; OCHO; X = (un)substituted hydrocarbon chain with optional heteroatoms; R4 = H, alkyl, (hetero)aryl; R5, R6 = H, alkyl; or R4R5 forms ring; n = undefined; Ar = (un)substituted (hetero)aryl; several addnl. provisos] were prepd. as inhibitors of 5-lipoxygenase, useful for treating inflammation, allergy, etc. For example, a mixt. of 2-thiopheneacetic acid, piperidine, and 3,5-dimethyl-4-hydroxybenzaldehyde (prepn. given) was refluxed with removal of H2O to give 61% dimethyl(thienylethenyl)phenol II. At 30 mg/kg i.p. in guinea pigs, II gave 75% inhibition of antigen-induced, leukotriene-mediated bronchoconstriction. I also inhibited inflammatory cell infiltration and LTB4 generation in animal expts.
IT 125722-37-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of lipoxygenase-inhibiting arylethenylphenol derivs.)
RN 125722-37-4 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-hydroxy-3,5-dimethylphenyl)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 152 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:594686 CAPLUS
DOCUMENT NUMBER: 111:194686
TITLE: A potent, tissue-selective, synthetic inhibitor of HMG-CoA reductase
AUTHOR(S): Balasubramanian, N.; Brown, P. J.; Catt, J. D.; Han, W. T.; Parker, R. A.; Sit, S. Y.; Wright, J. J.
CORPORATE SOURCE: Cardiovasc. Div., Bristol Myers Co., Wallingford, CT, 06492, USA
SOURCE: Journal of Medicinal Chemistry (1989), 32(9), 2038-41
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:194686
GI



AB (Tetrazolyl)bis(fluorophenyl)butadienylhydroxypyranone I was prepared and tested for 3-hydroxy-3-methylglutaryl CoA (HMG-CoA) reductase inhibitory activity. (4R,6S)-I and racemic I showed activity.
IT 118875-13-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to acid chloride)
RN 118875-13-1 CAPLUS
CN 1H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-1-methyl- (9CI) (CA INDEX NAME)



L4 ANSWER 152 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

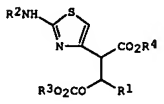
L4 ANSWER 153 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

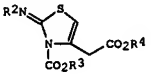
ACCESSION NUMBER: 1989:231619 CAPLUS
DOCUMENT NUMBER: 110:231619
TITLE: Preparation of aminothiazole derivatives as cephalosporin antibiotic intermediates
INVENTOR(S): Kinast, Guenther
PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.
SOURCE: Can., 42 pp. Division of Can. 1,212,949.
CODEN: CAXXA4
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 1238911	A2	19880705	CA 1986-505254	19860326
DE 3145727	A1	19830526	DE 1981-3145727	19811119
CA 1212949	A1	19861021	CA 1982-415708	19821117
CA 1240985	A2	19880823	CA 1987-541405	19870706
CA 1247109	A2	19881220	CA 1987-541321	19870706

PRIORITY APPLN. INFO.: DE 1981-3145727 A 19811119
CA 1982-415708 A3 19821117
CA 1986-505254 A3 19860326

OTHER SOURCE(S): CASREACT 110:231619; MARPAT 110:231619
GI


I


II

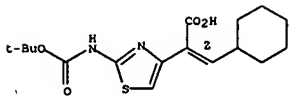
AB The title compds. [I; R1 = (substituted) alkyl, cycloalkyl, (hetero)aryl; R2 = CO2R3; R3, R4 = alkyl, alkenyl, cycloalkyl, cycloalkenyl, (hetero)aryl], useful as intermediates for cephalosporin antibiotics, were prepared from iminothiazolineacetates II. A mixture of Et 2-[(tert-butoxycarbonyl)imino]-3-(tert-butoxycarbonyl)-4-thiazoline-4-acetate, BuLi, and AcH in THF was stirred 2 h at -50 to -60° to give Et 2-[2-[(tert-butoxycarbonyl)amino]thiazol-4-yl]-3-[(tert-butoxycarbonyl)oxybutyrate.

IT 86978-31-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antibiotic intermediate)

RN 86978-31-6 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclohexylmethylene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

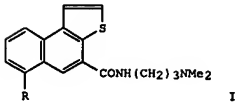
L4 ANSWER 153 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



L4 ANSWER 154 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

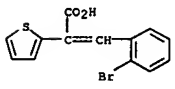
ACCESSION NUMBER: 1989:212529 CAPLUS
DOCUMENT NUMBER: 110:212529
TITLE: Synthesis of N-(3-dimethylaminopropyl)-6-substituted naphtho[2,1-b]thiophene-4-carboxamides
AUTHOR(S): Ming, Yang; Boykin, David W.
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, GA, 30303-3083, USA
SOURCE: Journal of Heterocyclic Chemistry (1988), 25(6), 1729-31
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:212529
GI


I

AB N-(3-Dimethylaminopropyl)-6-substituted naphtho[2,1-b]thiophenes-4-carboxamides I (R = OMe, Me, F, Cl, Br, CF3, cyano) were synthesized starting from 2-RC6H4CHO and 2-thiopheneacetic acid. Six substituted naphtho[2,1-b]thiophene-4-carboxylic acids were obtained upon oxidative-photocyclization of α-(2-thienyl)-β-arylacrylic acids. The naphtho[2,1-b]thiophenecarboxylic acids were converted to the corresponding amides through their acid chlorides or, in one case, by use of 1,1-carbonyldiimidazole coupling of the amine and the acid.

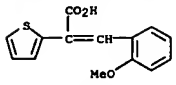
IT 115978-63-7P 120616-38-8P 120616-39-9P
120616-40-2P 120616-41-3P 120616-42-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photochem. cyclization of)

RN 115978-63-7 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2-bromophenyl)methylene]- (9CI) (CA INDEX NAME)

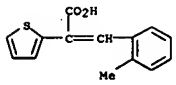


RN 120616-38-8 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

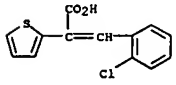
L4 ANSWER 154 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



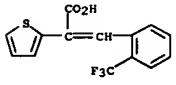
RN 120616-39-9 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2-methylphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 120616-40-2 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)

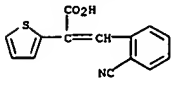


RN 120616-41-3 CAPLUS
CN 2-Thiopheneacetic acid, α-[[2-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 120616-42-4 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2-cyanophenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 154 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 155 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

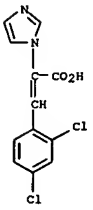
ACCESSION NUMBER: 1989:173227 CAPLUS
DOCUMENT NUMBER: 110:173227
TITLE: Preparation of α-imidazolyl-γ-phenylpropionate derivatives and their metal complexes as agrochemical microbicides.
INVENTOR(S): Ishii, Teruhiko; Kimata, Toshiya; Hayashi, Shunji; Motoyoshi, Masatoshi; Yamaguchi, Matsutaro
PATENT ASSIGNEE(S): SDS Biotech K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63072678	A	19880402	JP 1986-217222	19860917
PRIORITY APPLN. INFO.:			JP 1986-217222	19860917

OTHER SOURCE(S): CASREACT 110:173227
GI

AB Title compds. I [R = (halo-, Me-, MeO-, or O2N-substituted)Ph; R1, R2 = C1-8 alkyl, C4-8 cycloalkyl; Y = O, S, NR3; Z = O, S, NR4; R3, R4 = H, C1-8 alkyl, C4-8 cycloalkyl, aralkyl; R1R4N, R2R3N = heterocyclyl; except when Z = S, Y=O] and their metal complexes are prepared as agrochem. microbicides. Treatment of 2',4'-dichloro-2-(1-imidazolyl)cinnamic acid with SOCl2, followed by amidation of the acid chloride with Et2NH in CH2Cl2 gave 86% N,N-diethyl-2',4'-dichloro-2-(1-imidazolyl)cinnamamide, which in EtOH was treated with EtSH in the presence of piperidine to afford 74% I (R = 2,4-Cl2C6H3; R1Z = EtS; R2Y = Et2N) (II). II at 20 ppm showed 100% control of Sphaerotheca fuliginea. An emulsion was formulated containing 20 g I, 10 g Sorpol 2680, in 100 mL xylene.
IT 118851-74-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of imidazolyl (phenyl)propionate microbicides)
RN 118851-74-4 CAPLUS
CN 1H-Imidazole-1-acetic acid, α-[(2,4-dichlorophenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 155 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 156 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:154302 CAPLUS
DOCUMENT NUMBER: 110:154302
TITLE: Preparation of 5-(2,2-diphenylethenyl)1-methyl-1H-tetrazoles as intermediates for anticholesteremics
INVENTOR(S): Wright, John J.; Sit, Sing Yuen; Balasubramanian, Neelakantan; Brown, Peter J.
PATENT ASSIGNEE(S): Bristol-Myers Co., USA
SOURCE: Ger. Offen., 41 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3805789	A1	19880915	DE 1988-3805789	19880224
DE 3805789	C2	20010531		
US 4898949	A	19900206	US 1988-151512	19880218
DK 8800973	A	19880826	DK 1988-973	19880224
FI 8800868	A	19880826	FI 1988-868	19880224
FI 96600	B	19960415		
FI 96600	C	19960725		
FR 2611201	A1	19880826	FR 1988-2212	19880224
FR 2611201	B1	19910111		
NO 8800802	A	19880826	NO 1988-802	19880224
NO 178432	B	19951218		
NO 178432	C	19960327		
SE 8800637	A	19880826	SE 1988-637	19880224
SE 504553	C2	19970303		
AU 8812132	A	19880901	AU 1988-12132	19880224
AU 610562	B2	19910523		
NL 8800468	A	19880916	NL 1988-468	19880224
GB 2202845	A	19881005	GB 1988-4281	19880224
GB 2202845	B	19910522		
ZA 8801278	A	19881026	ZA 1988-1278	19880224
JP 63290872	A	19881128	JP 1988-41828	19880224
HU 47258	A2	19890228	HU 1988-885	19880224
HU 201532	B	19901128		
ES 2009547	A6	19891001	ES 1988-533	19880224
HU 201533	B	19901128	HU 1989-5124	19880224
HU 201534	B	19901128	HU 1989-5133	19880224
CH 678182	A5	19910815	CH 1988-691	19880224
CS 274669	B2	19910915	CS 1988-1181	19880224
CS 274690	B2	19910915	CS 1989-2768	19880224
CS 274691	B2	19910915	CS 1989-2769	19880224
CS 274692	B2	19910915	CS 1989-2770	19880224
CS 274693	B2	19910915	CS 1989-2771	19880224
AT 8800460	A	19920615	AT 1988-460	19880224
AT 395588	B	19930125		
CA 1328269	C	19940405	CA 1988-559671	19880224
CN 88100993	A	19880907	CN 1988-100993	19880225
CN 1022564	B	19931027		
BE 1002115	A3	19900710	BE 1988-219	19880225
DD 297818	A5	19920123	DD 1988-313193	19880225

L4 ANSWER 156 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

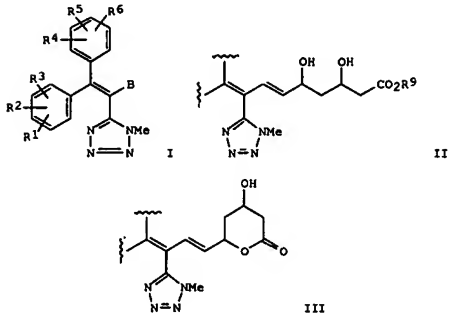
US 4939265	A	19900703	US 1989-430029	19891101
AT 9200380	A	19951215	AT 1992-380	19920228
AT 401263	B	19960725		
AT 9200381	A	19951215	AT 1992-381	19920228
AT 401264	B	19960725		
CN 1070642	A	19930407	CN 1992-111551	19921020
CN 1030077	B	19951018		
NO 9204941	A	19880826	NO 1992-4941	19921221
NO 179207	C	19960828		
NO 9204942	A	19880826	NO 1992-4942	19921221
NO 178190	B	19951030		
NO 178190	C	19960207		
SE 503201	C2	19960415	SE 1993-976	19930324
SE 512485	C2	20000320	SE 1993-977	19930324
FI 96602	B	19960415	FI 1993-1580	19930407
FI 96602	C	19960725		
FI 96953	B	19960614	FI 1993-1579	19930407
FI 96953	C	19960925		
NO 178767	B	19960219	NO 1994-2083	19940606
NO 178767	C	19960529		
DK 9701138	A	19971006	DK 1997-1138	19971006

PRIORITY APPLN. INFO.:

US 1987-18558	A	19870225
US 1988-151512	A	19880218
AT 1988-460	A	19880224
NO 1988-802	A1	19880224
CN 1988-100993	A	19880225

OTHER SOURCE(S): MARPAT 110:154302
GI

L4 ANSWER 156 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

II

III

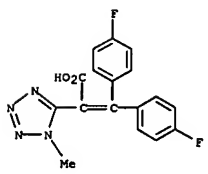
AB The title compds [I; B = H, C1-6 alkoxycarbonyl, RCH2; R = H, OH, (R7O)2P(O), P+R83 X-; R1, R4 = CF3, R2; R2, R3, R5, R6 = H, C1-4 alkyl, C1-4 alkoxy, halo; R7 = C1-4 alkyl; R8 = (un)substituted Ph; X = Br, Cl, iodo] were prepared as intermediates for anticholesteremic (no data) dihydroxy(tetrazolyl)nonadienoates II (R9 = H, hydrolyzable ester group, pharmaceutically acceptable cation) and their corresponding δ-lactones III. 1,5-Dimethyltetrazole was treated with BuLi and MeI at -78° to give 5-ethyl-1-methyltetrazole which was lithiated and condensed with (4-FC6H4)2CO to give, after dehydration, I (R1 = R4 = F, R2 = R3 = R5 = R6 = H, B = Me). The latter was converted in 3 steps to I (B = CH2P+Ph3 Br-, other groups unchanged) which underwent a Wittig reaction with Me erythro-3,5-bis(tert-butyldimethylsiloxy)-6-oxohexanoate to give, after deprotection, (±)-erythro-II (R9 = Me, R1-R6 as given previously).

IT 118875-13-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anticholesteremic intermediate)

RN 118875-13-1 CAPLUS

CN 1H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-1-methyl- (9CI) (CA INDEX NAME)

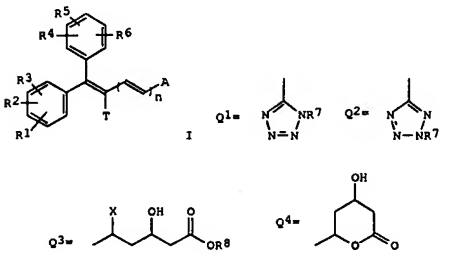
L4 ANSWER 156 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 157 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:114836 CAPLUS
DOCUMENT NUMBER: 110:114836
TITLE: Preparation and testing of tetrazolyldiarylalkenoates as antihypercholesteremics
INVENTOR(S): Wright, John J.; Sit, Sing Yuen
PATENT ASSIGNEE(S): Bristol-Myers Co., USA
SOURCE: Ger. Offen., 104 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

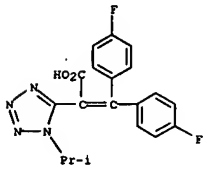
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3805801	A1	19880908	DE 1988-3805801	19880224
DE 3805801	C2	20010301		
US 4897490	A	19900130	US 1988-151513	19880218
PRIORITY APPLN. INFO.:			US 1987-18542 A	19870225
			US 1988-151513 A	19880218

OTHER SOURCE(S): MARPAT 110:114836
GI

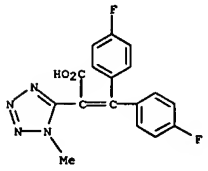


AB The title compds. (I; R1, R4 = H, halo, C1-4 alkyl, alkoxy, CF3; R2, R3, R5, R6 = H, halo, C1-4 alkyl, alkoxy:; R7 = H, C1-4 alkyl, alkoxyalkyl, methoxyethoxymethyl; R8 = H, cation, hydrolyzable ester group; A = Q3, Q4; T = Q1, Q2; X = OH, :O; n = 0-2) useful as antihypercholesteremics, were prepared 3,3-Bis(4-fluorophenyl)-2-(1-methyl-1H-tetrazol-5-yl)-2-propenal

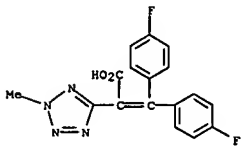
L4 ANSWER 157 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(prepn. of. as intermediate for antihypercholesteremic)
RN 118845-64-0 CAPLUS
CN 1H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-1-(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 157 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(prepn. given) and Ph3P:CH2CHO were refluxed 30 min in C6H6 to give 89% of the corresponding pentadienal (contaminated by .apprx.10% of heptatrienal). The pentadienal in THF was treated with Et acetoacetate in THF at -78° to give 58% Et 9,9-bis(4-fluorophenyl)-5-hydroxy-8-(1-methyl-1H-tetrazol-5-yl)-3-oxo-6,8-nonadienoate. The latter in THF was treated with Et3B in THF and then with NaBH4 at -78° to give 68% of the 3,5-dihydroxy ester, which was sapond. with 1N NaOH in THF to give 100% Na (±)-erythro-9,9-bis(4-fluorophenyl)-3,5-dihyudroxy-8-(1-methyl-1H-tetrazol-5-yl)-6,8-nonadienoate (II). II inhibited cholesterol biosynthesis in isolated rat hepatocytes with an IC50 of 23.0 nM, vs. 46.0 nm for mevinolin.
IT 118875-13-1P 118875-14-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antihypercholesteremic)
RN 118875-13-1 CAPLUS
CN 1H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-1-methyl- (9CI) (CA INDEX NAME)



RN 118875-14-2 CAPLUS
CN 2H-Tetrazole-5-acetic acid, α-[bis(4-fluorophenyl)methylene]-2-methyl- (9CI) (CA INDEX NAME)

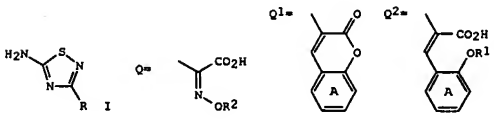


IT 118845-64-0
RL: RCT (Reactant); RACT (Reactant or reagent)

L4 ANSWER 158 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:631026 CAPLUS
DOCUMENT NUMBER: 109:231026
TITLE: Preparation of 2-(5-amino-1,2,4-thiadiazol-3-yl)-2-(hydroxy- or alkoxyimino)acetic acids for acylating amino groups of cephalosporins, penicillins and azetidinones
INVENTOR(S): Yamaoka, Masayoshi; Hashimoto, Naoto
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62205066	A	19870909	JP 1986-47694	19860304
JP 06096562	B	19941130		
PRIORITY APPLN. INFO.:			JP 1986-47694	19860304

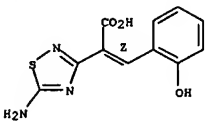
GI



AB The title compds. [I; R = Q; R2 = H, (un)substituted alkyl] (II) were prepared in several steps starting from I (R = Q1, benzene ring A being optionally substituted) (III). A suspension of 3-(5-amino-1,2,4-thiadiazol-3-yl)coumarin (IV) in EtOH was treated with 1N NaOH for 60 min. After adding EtOAc and neutralizing with 1N HCl under ice-cooling, the EtOAc layer containing 2-(5-amino-1,2,4-thiadiazol-3-yl)-2(Z)-(2-hydroxybenzylidene)acetic acid (V) was separated and treated with O3 at -78°. H2O was added to the mixture and vigorously stirred to give an aqueous solution of I [R = C(O)CO2H] (VI) which was reacted with MeONH2.HCl and AcONa for 3 h at room temperature to give I (R = Q, R2 = Me).
IT 117510-25-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, by Et chloroformate)
RN 117510-25-5 CAPLUS
CN 1,2,4-Thiadiazole-3-acetic acid, 5-amino-α-[(2-hydroxyphenyl)methylene]-, disodium salt, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

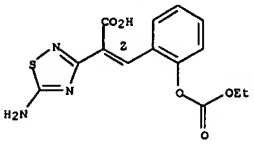
L4 ANSWER 158 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



●2 Na

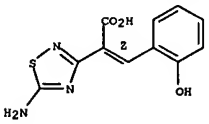
IT 117510-26-6P 117510-27-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ozonolysis of)
RN 117510-26-6 CAPLUS
CN 1,2,4-Thiadiazole-3-acetic acid, 5-amino-α-[[2-[(ethoxycarbonyl)oxy]phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 117510-27-7 CAPLUS
CN 1,2,4-Thiadiazole-3-acetic acid, 5-amino-α-[(2-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

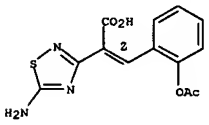
Double bond geometry as shown.



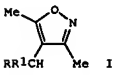
IT 117510-22-2P

L4 ANSWER 158 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for (aminothiadiazolyl)(alkoxyimino)acetic acid)
RN 117510-22-2 CAPLUS
CN 1,2,4-Thiadiazole-3-acetic acid, α-[[2-(acetyloxy)phenyl]methylene]-5-amino-, (Z)- (9CI) (CA INDEX NAME)

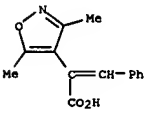
Double bond geometry as shown.



L4 ANSWER 159 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:528874 CAPLUS
DOCUMENT NUMBER: 109:128874
TITLE: Production and transformation of carbanion derivatives of C-4α-functionalized 3,5-dimethylisoxazoles
AUTHOR(S): Alberola, A.; Alonso, F.; Banez, M.; Cuadrado, P.; Mocha, F. A.; Sanudo, M. C.
CORPORATE SOURCE: Dep. Quim. Org., Univ. Valladolid, Valladolid, 47011, Spain
SOURCE: Anales de Quimica, Serie C: Quimica Organica y Bioquimica (1987), 83(2), 182-94
CODEN: AQSBD6; ISSN: 0211-1357
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
OTHER SOURCE(S): CASREACT 109:128874
GI

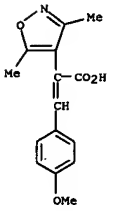


AB Methylisoxazoles I (R = H, R1 = CN, CO2Et, CO2CMe3, tosyl; R = Ph, R1 = tosyl) are deprotonated by bases at the C-4α position. The resulting carbanions undergo alkylation, acylation, 1,2-addition, or Michael-type addition to afforded 4α-substituted isoxazoles. The reaction are highly dependent on steric hindrance at C-4α.
IT 116422-78-7P 116422-79-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 116422-78-7 CAPLUS
CN 4-Isoxazoleacetic acid, 3,5-dimethyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

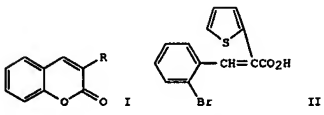


RN 116422-79-8 CAPLUS
CN 4-Isoxazoleacetic acid, α-[(4-methoxyphenyl)methylene]-3,5-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 159 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

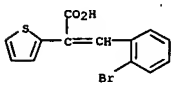


L4 ANSWER 160 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:492553 CAPLUS
DOCUMENT NUMBER: 109:92553
TITLE: A convenient synthesis of 3-arylcoumarins
AUTHOR(S): Ming, Yang; Boykin, David W.
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, GA, 30303, USA
SOURCE: Heterocycles (1987), 26(12), 3229-31
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:92553
GI

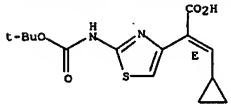


I II

AB 3-Arylcoumarins I (R = 2-thienyl, 3-thienyl, Ph, 4-ClC6H4, 4-MeC6H4) were obtained in 27-47% yield by treating 2-FC6H4CHO with RCH2CO2H in the presence of Et3N.
IT 115978-63-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 115978-63-7 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2-bromophenyl)methylene]- (9CI) (CA INDEX NAME)

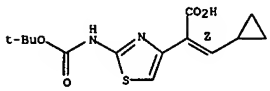


L4 ANSWER 161 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 114569-61-8 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclopropylmethylene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

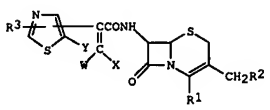
Double bond geometry as shown.



L4 ANSWER 161 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:221491 CAPLUS
DOCUMENT NUMBER: 108:221491
TITLE: Preparation of alkenylcarboxamidocephemcarboxylic acid derivatives as antibiotics
INVENTOR(S): Takatani, Takao; Sakane, Kazuo; Yamanaka, Hideaki; Matsuo, Teruaki
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62215593	A	19870922	JP 1986-58860	19860317
PRIORITY APPLN. INFO.:			JP 1986-58860	19860317

GI



I

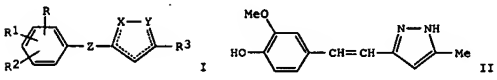
AB The title compds. I [R1 = (protected) CO2H, CO2-; R3 = (protected) amino; Y = H, halo; one of W and X is H, the other is Me, MeSCH2, cycloalkyl, pyrazolyl, tetrazolyl, 2-oxodihydropyridyl, etc.; R2 = pyridino, thiazolylthio, alkyl-substituted tetrazolylthio; with the proviso that Y is halo when one of W and X is H and the other is Me; when R1 = CO2-, R2 is pyridinio], useful as antibiotics (no data), were prepared Condensation of 1-(2-tert-butoxycarbonylamino-5-chlorothiazol-4-yl)-1-(Z)-propenecarboxylic acid (preparation given) with 7-amino-3-pyridiniummethyl-3-cephem-4-carboxylic acid-2HCl, followed by deprotection in PhOMe/CF3CO2H gave 7-[1-(2-amino-5-chlorothiazol-4-yl)]-1-(Z)-propenecarboxamido-3-pyridiniummethyl-3-cephem-4-carboxylate.
IT 114569-60-7P 114569-61-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as cephalosporin antibiotic intermediate)
RN 114569-60-7 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclopropylmethylene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 162 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:131808 CAPLUS
DOCUMENT NUMBER: 108:131808
TITLE: Preparation of novel styrylpyrazoles, styrylisoxazoles, and analogs as 5-lipoxygenase inhibitors
INVENTOR(S): Belliotti, Thomas R.; Connor, David T.; Flynn, Daniel L.; Kostlan, Catherine R.; Nies, Donald E.
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: Eur. Pat. Appl., 58 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 245825	A1	19871119	EP 1987-106822	19870511
EP 245825	B1	19910313		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 8771973	A	19871112	AU 1987-71973	19870424
AU 613579	B2	19910808		
ZA 8702997	A	19881228	ZA 1987-2997	19870427
DK 8702269	A	19871110	DK 1987-2269	19870504
DK 175824	B1	20050314		
CA 1330442	C	19940628	CA 1987-536430	19870505
FI 8702015	A	19871110	FI 1987-2015	19870506
NO 8701917	A	19871110	NO 1987-1917	19870508
JP 63022079	A	19880129	JP 1987-110955	19870508
AT 61582	T	19910315	AT 1987-106822	19870511
ES 2037681	T3	19930701	ES 1987-106822	19870511
US 4877881	A	19891031	US 1988-247837	19880921
US 4924002	A	19900508	US 1989-310260	19890213
US 5208251	A	19930504	US 1989-395165	19890816
PRIORITY APPLN. INFO.:			US 1986-861179 A	19860509
			US 1986-910692 A	19860922
			US 1987-32730 A	19870406
			EP 1987-106822 A	19870511

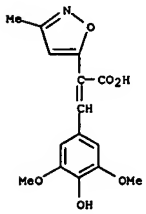
OTHER SOURCE(S): CASREACT 108:131808; MARPAT 108:131808
GI



I II

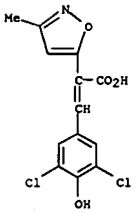
AB The title compds. [I, R-R2 = H, alkyl, HOCH2, CF3, R4O, R5S, NO2, R4CO2, R4CO, CO2R5, R6R7N, R4CONH, HCONH, R4SO2NH, R5NHCONH; R3 = H, alkyl, CF3, (hetero)aryl, (hetero)aralkyl, halo, R4CO2, R4CO, CO2R5, R6O2CCHR7, RR1R2C6H2CH:CH; R4 = alkyl; R5-R7 = H, alkyl; X, Y = O, S, N, R8N; R8 = H,

L4 ANSWER 162 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
alkyl, R6O2CCHR7, R5CO, C3-20 cycloalkyl, aryl, aralkyl; Z = (CH2)n, CH:CH, CH:C(CO2R5); dotted line indicates 2 conjugated double bonds in azole ring) were prepd. as inhibitors of 5-lipoxygenase and cycloxygenase,
useful as antiinflammatories, allergy inhibitors, and as sunscreens. 4,6-HO(MeO)C6H3CHO and CH2(COMe)2 were stirred at room temp. in EtOAc contg. B2O3 to give 90% 4,6-HO(MeO)C6H3CH:CHCOCH2COMe. The latter was cyclocondensed with N2H4.H2O in EtOH/BuOH contg. HOAc to give 53% styrylpyrazole II. II inhibited 5-lipoxygenase and cyclooxygenase of rat basophilic leukemia cells with IC50 of 0.8 μM and 13.0 μM, resp.
IT 113465-45-5P 113465-46-6P 113465-47-7P
113465-48-8P 113465-49-9P 113465-50-2P
113465-51-3P 113465-52-4P 113465-60-4P
113465-61-5P 113465-62-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as drug)
RN 113465-45-5 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3,5-dimethoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

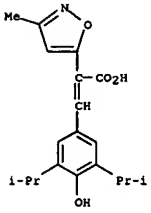


RN 113465-46-6 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(3,5-dichloro-4-hydroxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 162 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

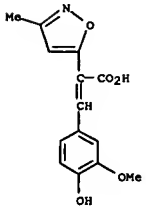


RN 113465-47-7 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3,5-bis(1-methylethyl)phenyl]methylene]-3-methyl- (9CI) (CA INDEX NAME)

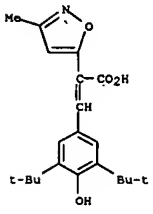


RN 113465-48-8 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3-methoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 162 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

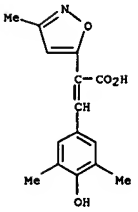


RN 113465-49-9 CAPLUS
CN 5-Isoxazoleacetic acid, α-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]-3-methyl- (9CI) (CA INDEX NAME)

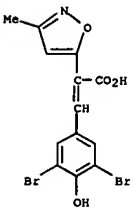


RN 113465-50-2 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(4-hydroxy-3,5-dimethylphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 162 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

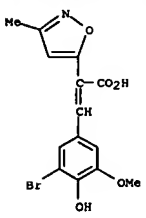


RN 113465-51-3 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(3,5-dibromo-4-hydroxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

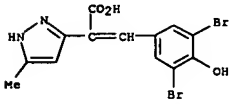


RN 113465-52-4 CAPLUS
CN 5-Isoxazoleacetic acid, α-[(3-bromo-4-hydroxy-5-methoxyphenyl)methylene]-3-methyl- (9CI) (CA INDEX NAME)

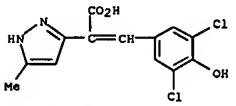
L4 ANSWER 162 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 113465-60-4 CAPLUS
CN 1H-Pyrazole-3-acetic acid, α-[(3,5-dibromo-4-hydroxyphenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)

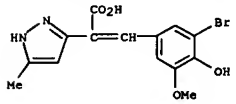


RN 113465-61-5 CAPLUS
CN 1H-Pyrazole-3-acetic acid, α-[(3,5-dichloro-4-hydroxyphenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)

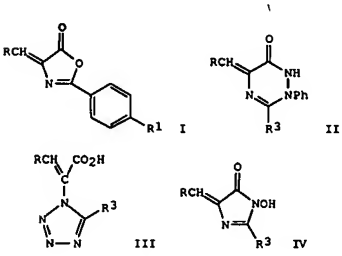


RN 113465-62-6 CAPLUS
CN 1H-Pyrazole-3-acetic acid, α-[(3-bromo-4-hydroxy-5-methoxyphenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 162 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 163 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:439707 CAPLUS
DOCUMENT NUMBER: 107:39707
TITLE: Synthesis and reactions of some 2-aryl-4-arylidene-5(4)-oxazolones
AUTHOR(S): Afifi, A. A.; Salem, M. A. I.; El-Hashash, M. A.; El-Kady, S. S.
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
SOURCE: Journal of the Chemical Society of Pakistan (1986), 8(3), 297-304
CODEN: JCSPDF; ISSN: 0253-5106
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:39707
GI

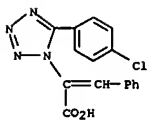


AB The title compds. I (R = e.g. Ph, 3-ClC6H4, 4-O2NC6H4, 4-Me2NC6H4; R1 = Me, Cl, NO2) reacted with amines and hydrazines in EtOH to give arylacrylamides 4-R1C6H4CONHC(:CHR)CONHR2 (R2 = alkyl, aryl, cyclohexyl, PhCH2, NH2, NHPh). Reaction of I with PhNHNH2 and NaN3 in AcOH, and with NH2OH.HCl in pyridine gave triazines II (R3 = 4-R1C6H4), tetrazoles III and imidazoles IV, resp. Reaction of IV with PhNHNH2 yielded II.

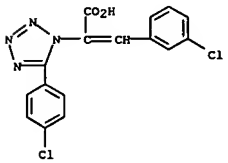
IT 90125-21-6P 90125-22-7P 90125-23-8P
90125-24-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 90125-21-6 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(4-chlorophenyl)-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

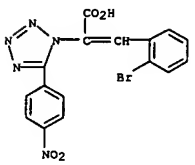
L4 ANSWER 163 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 90125-22-7 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(4-chlorophenyl)-α-[(3-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)

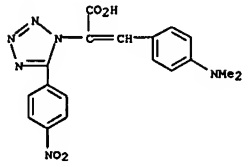


RN 90125-23-8 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[(2-bromophenyl)methylene]-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 90125-24-9 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[[4-(dimethylamino)phenyl]methylene]-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 163 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 164 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

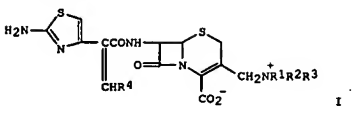
ACCESSION NUMBER: 1986:626175 CAPLUS
DOCUMENT NUMBER: 105:226175
TITLE: β-Lactam antibiotics and their use as a drug or growth promoter in animal husbandry or as an antioxidant
INVENTOR(S): Angerbauer, Rolf; Boberg, Michael; Metzger, Karl; Zeiler, Hans Joachim
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 69 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3419012	A1	19851128	DE 1984-3419012	19840522
CN 85101682	A	19870131	CN 1985-101682	19850401
US 4632918	A	19861230	US 1985-730979	19850506
EP 163190	A2	19851204	EP 1985-105841	19850513
EP 163190	A3	19861126		
EP 163190	B1	19900411		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 51870	T	19900415	AT 1985-105841	19850513
AU 8542564	A	19851128	AU 1985-42564	19850516
AU 572994	B2	19880519		
JP 60255795	A	19851217	JP 1985-104108	19850517
CA 1274821	A1	19901002	CA 1985-481749	19850517
FI 8502003	A	19851123	FI 1985-2003	19850520
ES 543300	A1	19860601	ES 1985-543300	19850520
IL 75239	A	19900429	IL 1985-75239	19850520
IL 88528	A	19900429	IL 1985-88528	19850520
DK 8502262	A	19851123	DK 1985-2262	19850521
ZA 8503829	A	19860129	ZA 1985-3829	19850521
HU 38648	A2	19860630	HU 1985-1914	19850521
HU 193760	B	19871130		
ES 552571	A1	19871201	ES 1986-552571	19860228
ES 552572	A1	19880716	ES 1986-552572	19860228
ES 552572	A5	19880812		
ES 557783	A1	19880416	ES 1987-557783	19871215
AU 8811989	A	19880609	AU 1988-11989	19880217
AU 593460	B2	19900208		

PRIORITY APPLN. INFO.:	DE 1984-3419012		19840522
	EP 1985-105841	A	19850513
	IL 1985-75239	A	19850520

OTHER SOURCE(S): CASREACT 105:226175; MARPAT 105:226175
GI

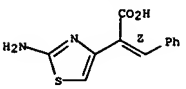
L4 ANSWER 164 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

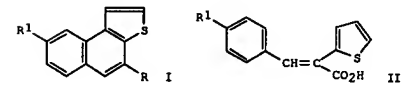
AB β-Lactam compds. I [(R1, R2, R3 = (un)substituted alkyl or mono- or bicyclic carbo- or heterocyclyl; R1 as given, R2R3N (un)substituted mono or polycyclic ring and may contain O, S, and N as further hetero atoms; R1R3R3N = bridged (un)substituted polycyclic ring and may contain O, S, and N as further hetero atoms; R4 = H, (un)substituted alkyl, aryl, heterocyclyl, CO2H, alkoxycarbonyl, halo, pseudohalo, ABS(O)n [n = 0-2; B = bond, O, NW; A, W = H, (un)substituted alkyl, aryl, heterocyclyl; AW form a carbocycle or heterocyclic ring]], useful as antioxidants, antibacterials, and animal growth promoters (no data), were prepared 7-[1-(2-Amino-4-thioazolyl)-1(Z)-propenecarboxyamido]-3-(1-methyl-1-pyrrolidinio)methyl-3-cephem-4-carboxylate was prepared in 4 steps from benzhydryl 3-(hydroxymethyl-7β-phenylacetamido-3-cephem-4-carboxylate and SOCl2.
IT 82617-91-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of aminocephemcarboxylate derivative)
RN 82617-91-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(phenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 165 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

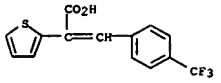
ACCESSION NUMBER: 1986:533695 CAPLUS
DOCUMENT NUMBER: 105:133695
TITLE: Synthesis of 8-substituted naphtho[2,1-b]thiophenes with cationic side chains at position 4
AUTHOR(S): Kusuma, Srihari; Wilson, W. David; Boykin, David W.
CORPORATE SOURCE: Lab. Microb. Biochem. Sci., Georgia State Univ., Atlanta, GA, 30303-3083, USA
SOURCE: Journal of Heterocyclic Chemistry (1985), 22(5), 1229-32
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:133695
GI



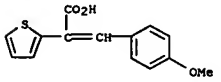
I II

AB Naphtho[2,1-b]thiophenes I [R = CH(OH)CH2N(CH2CH2OH)2; R1 = H, F, Cl, CF3, cyano] and naphtho[2,1-b]thiophene-4-carboxamides I [R = CONH(CH2)3NMe2; R1 = MeO, Me, H, F, Cl, CF3, cyano] were prepared The naphtho[2,1-b]thiophene-4-carboxylic acids I (R = CO2H) were prepared by photooxidative cyclization of α-(2-thienyl)-β-arylacrylic acids II. The carboxylic acids I (R = CO2H) were converted by a conventional 5-step route involving α-bromo ketone intermediates to the naphtho[2,1-b]thiophene-4-methanols I [R = CH(OH)CH2N(CH2CH2OH)2] and by a standard 2-step amide preparation to the naphtho[2,1-b]thiophene-4-carboxamides I [R = CONH(CH2)3NMe2].
IT 37094-47-6P 104314-01-4P 104314-02-5P 104314-03-6P 104314-04-7P 104314-05-8P 104314-06-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photocyclization of, naphthothiophenecarboxylic acids from)
RN 37094-47-6 CAPLUS
CN 2-Thiopheneacetic acid, α-[[4-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)

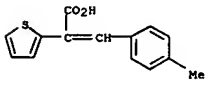
L4 ANSWER 165 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



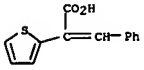
RN 104314-01-4 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 104314-02-5 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)

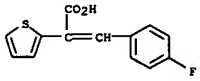


RN 104314-03-6 CAPLUS
CN 2-Thiopheneacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)

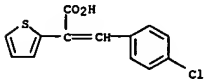


RN 104314-04-7 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-fluorophenyl)methylene]- (9CI) (CA INDEX NAME)

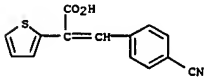
L4 ANSWER 165 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 104314-05-8 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)



RN 104314-06-9 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-cyanophenyl)methylene]- (9CI) (CA INDEX NAME)

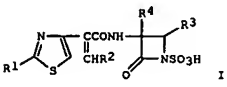


L4 ANSWER 166 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:533653 CAPLUS
DOCUMENT NUMBER: 105:133653
TITLE: 3-Acylamino-2-aztidinone-1-sulfonic and derivatives
INVENTOR(S): Matsumura, Kiyotoshi; Akagi, Hiroshi; Kyokawa, Hiroshi; Suzuki, Daisuke; Shimabayashi, Akihiro; Yonemoto, Yoshimasa
PATENT ASSIGNEE(S): Otsuka Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61024592	A	19860203	JP 1984-145798	19840712
PRIORITY APPLN. INFO.:			JP 1984-145798	19840712

OTHER SOURCE(S): CASREACT 105:133653
GI



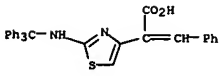
I

AB Title compds. I [R1 = (un)protected amino; R2 = H, (un)substituted Ph, heterocyclyl, alkyl, cycloalkyl, (esterified)carboxy, halo; R3 = H, alkyl; R4 = H, MeO] and their salts, useful as bactericides (min. inhibitory concentration given), were prepared Thus, stirring 0.15 g 3-amino-4-methyl-2-azetidinone-1-sulfonic acid with 0.31 g 3-phenyl-2-(2-tritylaminothiazol-4-yl)propenoic acid (Z-isomer), 0.12 mL NEt3, 0.17 g 1-hydroxybenzotriazole, and 0.17 g N,N-dicyclohexylcarbodiimide in DMF at room temperature for 15 h gave, after treatment with aqueous KHCO3, 89.6% 3-[2-benzylidene-2-(2-tritylaminothiazol-4-yl)acetamides)-4-methyl-2-azetidinone-1-sulfonic acid potassium salt (Z-isomer).

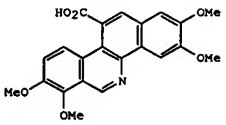
IT 104211-39-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)

RN 104211-39-4 CAPLUS
CN 4-Thiazoleacetic acid, α-(phenylmethylene)-2-[(triphenylmethyl)amino]- (9CI) (CA INDEX NAME)

L4 ANSWER 166 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



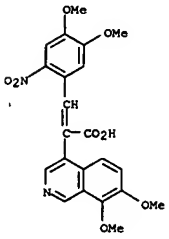
L4 ANSWER 167 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:523746 CAPLUS
DOCUMENT NUMBER: 103:123746
TITLE: Alkaloids. XLVIII. Attempts at the synthesis of 11-methoxy-substituted benzo[c]phenanthridines
AUTHOR(S): Smidrkal, Jan; Holubek, Jiri; Slanger, Jiri; Trojanek, Jan
CORPORATE SOURCE: Res. Inst. Pharm. Biochem., Prague, 194 04, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1985), 50(4), 861-8, 1 plate
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:123746
GI



I

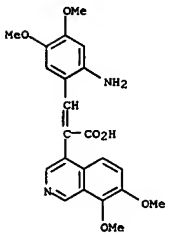
AB Expts. aimed at the synthesis of so far unknown 11-methoxybenzo[c]phenanthridines are described. In the first approach 2,3,7,8-tetramethoxybenzo[c]phenanthridine-11-carboxylic acid (I) was synthesized using a procedure for the preparation of 2,3,7,8-bismethylenedioxybenz[c]phenanthridine-11-carboxylic acid. Attempts to convert the carboxyl group of these acids to the methoxyl group were not successful. In the second approach 3-methoxy-6,7-methylenedioxy-1-methylaminonaphthalene was prepared from 1-(3,4-methylenedioxyphenyl)-2-propanone by a multistep synthesis. On acylation of the product with 2,3-dimethoxy-6-nitrobenzoic acid and subsequent hydrogenation N-(3-methoxy-6,7-methylenedioxynaphth-1-yl)-N-methylamide of 6-amino-2,3-dimethoxybenzoic acid was obtained. The attempts at its cyclization. according to Pschorr were unsuccessful.
IT 98263-39-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and diazotization-cyclization. of, benzophenanthridine derivative from)
RN 98263-39-9 CAPLUS
CN 4-Isoquinolineacetic acid, α-[(2-amino-4,5-dimethoxyphenyl)methylene]-7,8-dimethoxy-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 167 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

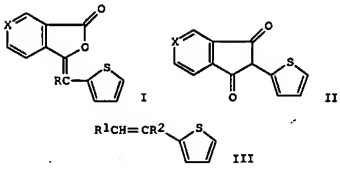
L4 ANSWER 167 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

IT 98263-38-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 98263-38-8 CAPLUS
CN 4-Isoquinolineacetic acid, α-[(4,5-dimethoxy-2-nitrophenyl)methylene]-7,8-dimethoxy-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 168 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:453897 CAPLUS
DOCUMENT NUMBER: 103:53897
TITLE: Reactions of 2-thienylacetic acid with anhydrides of dicarboxylic acids and aromatic aldehydes under the Perkin synthesis conditions
AUTHOR(S): Lacova, M.; Hrnciar, P.
CORPORATE SOURCE: Fac. Nat. Sci., Komensky Univ., Bratislava, CS-842 15, Czech.
SOURCE: Chemical Papers (1985), 39(1), 135-42
CODEN: CHPAEG; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

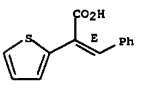


I II

III

AB 2-Thienylacetic acid underwent condensation with phthalic and 4-azaphthalic anhydride under conditions of the Gabriel modification of the Perkin synthesis to give adducts I (R = H, CO2H; X = CH, N). I (R = H, X = CH, N) rearranged to give indanone derivative II. Condensations of 2-thiopheneacetic acid with R1CHO (R1 = Ph, 2-thienyl, 3-ClC4H4, 4-ClC6H4, PhCH:CH) gave thiophenes III (R2 = H, or CO2H).
IT 38313-33-6P 97304-61-5P 97304-62-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38313-33-6 CAPLUS
CN 2-Thiopheneacetic acid, α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

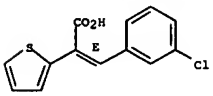
Double bond geometry as shown.



RN 97304-61-5 CAPLUS
CN 2-Thiopheneacetic acid, α-[(3-chlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

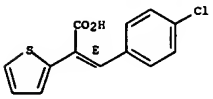
L4 ANSWER 168 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.

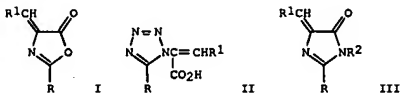


RN 97304-62-6 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-chlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

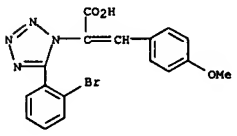
Double bond geometry as shown.



L4 ANSWER 169 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:591751 CAPLUS
DOCUMENT NUMBER: 101:191751
TITLE: Reaction of 2-aryl-4-arylidene-2-oxazolin-5-ones with some nucleophilic reagents
AUTHOR(S): Islam, A. M.; El-Sharief, A. M. S.; Ismail, I. M.; Harb, A. A.
CORPORATE SOURCE: Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1983), 26(3), 221-32
CODEN: EGJCA3; ISSN: 0367-0422
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:191751
GI

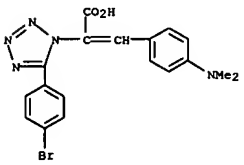


AB RCONHCH2CO2H [R = 2-BrC6H4, 4-BrC6H4, 3,5-(O2N)2C6H3], treated with R1CHO [R1 = Ph, 4-MeC6H4, 4-MeOC6H4, 4-Me2NC6H4, 3,4-(MeO)2C6H3, 2-thienyl], gave the title compds. (I), which were hydrolyzed with NaOH and NaOMe to give R1CH:C(CO2H)NHCOR and the Me ester, resp. Treatment of I with PhSH or NaN3 gave PhSCHR1CH(NHCOR)C(O)SPh and II, resp. I, treated with R2NH2 (R2 = 4-MeC6H4, PhCH2CH2, 2-furfuryl, cyclohexyl), in EtOH gave R1CH:C(NHCOR)CONHR2 and in AcOH gave imidazolinones III. III underwent sidechain substitution with PhCH2MgCl, but were cleaved by cyclohexylmagnesium bromide, BuMgBr, and MeMgI.
IT 92663-55-3P 92663-56-4P 92663-57-5P
92663-58-6P 92674-17-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 92663-55-3 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(2-bromophenyl)-α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

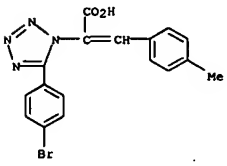


L4 ANSWER 169 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

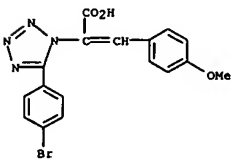
RN 92663-56-4 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(4-bromophenyl)-α-[[4-(dimethylamino)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 92663-57-5 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(4-bromophenyl)-α-[(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)

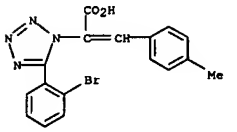


RN 92663-58-6 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(4-bromophenyl)-α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 92674-17-4 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(2-bromophenyl)-α-[(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 169 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



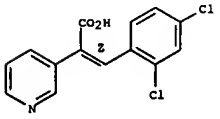
L4 ANSWER 170 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:423356 CAPLUS
DOCUMENT NUMBER: 101:23356
TITLE: Fungicidally active compositions containing ethylene derivatives
INVENTOR(S): Ten Haken, Pieter; Webb, Shirley Beatrice
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V., Neth.
SOURCE: Eur. Pat. Appl., 33 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 104690	A2	19840404	EP 1983-201249	19830830
EP 104690	A3	19850731		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
CA 1234388	A1	19880322	CA 1983-435095	19830822
DK 8304402	A	19840328	DK 1983-4402	19830926
DK 163703	B	19920330		
DK 163703	C	19920907		
FI 8303456	A	19840328	FI 1983-3456	19830926
FI 79930	B	19891229		
FI 79930	C	19900410		
NO 8303450	A	19840328	NO 1983-3450	19830926
NO 165221	B	19901008		
NO 165221	C	19910116		
AU 8319568	A	19840405	AU 1983-19568	19830926
AU 571458	B2	19880421		
BR 8305265	A	19840502	BR 1983-5265	19830926
JP 59078162	A	19840504	JP 1983-176543	19830926
JP 04046270	B	19920729		
ZA 8307141	A	19840530	ZA 1983-7141	19830926
HU 32485	A2	19840828	HU 1983-3333	19830926
HU 194481	B	19880229		
DD 213348	A5	19840912	DD 1983-255115	19830926
ES 525941	A1	19850416	ES 1983-525941	19830926
PL 136537	B1	19860228	PL 1983-243907	19830926
CS 259863	B2	19881115	CS 1983-6982	19830926
US 4600712	A	19860715	US 1985-785693	19851009

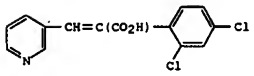
PRIORITY APPLN. INFO.: GB 1982-27480 A 19820927
US 1983-535496 A2 19830926

OTHER SOURCE(S): MARPAT 101:23356
GI

L4 ANSWER 170 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



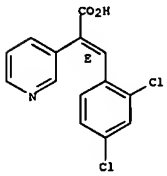
L4 ANSWER 170 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

AB Heterocyclic ethylenes RR1C:CR2R3 and RR3C:CR1R2 [R = 6-membered N heterocycle; R1 = H, (un)substituted alkyl; R2 = heterocycle, (un)substituted Ph; R3 = cyano, COR4; R4 = OH, Cl, alkoxy, alkylthio, (un)substituted NH2] were prepared Thus, 3-pyridinecarboxaldehyde was condensed with 2,4-C12C6H3CH2CO2H to give cis-I which at 1 kg/ha gave >80% control of Plasmopara viticola on vine plants.
IT 90750-44-0P 90750-74-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and fungicidal activity of)
RN 90750-44-0 CAPLUS
CN 3-Pyridineacetic acid, α-[(2,4-dichlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



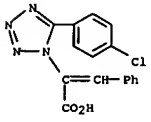
RN 90750-74-6 CAPLUS
CN 3-Pyridineacetic acid, α-[(2,4-dichlorophenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 171 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:191770 CAPLUS
DOCUMENT NUMBER: 100:191770
TITLE: Synthesis and reactions of some 2-aryl-4-arylidene-5(4)-oxazolones
AUTHOR(S): Afifi, A. A.; El Hashash, M. A.; El Kady, S. S.
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
SOURCE: Revue Roumaine de Chimie (1983), 28(8), 849-55
CODEN: RRCHAX; ISSN: 0035-3930
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:191770
GI

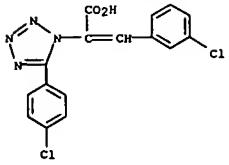
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Oxazolones I (R = Cl, R1, H, 3-Cl, 4-NO2, 4-NMe2; R = Me, R1 = 2-Cl, 4-Cl, 3-NO2; R = NO2, R1 = 4-NMe2; X = O) (II), prepared from R1C6H4CHO and 4-RC6H4CONHCH2CO2H, reacted with amines in EtOH to give acrylamides III (R2 = Bu, cyclohexyl, CH2Ph, 3,4-Me2C6H3, 2,5-MeClC6H3, 2-, 4-H2NC6H4) and IV (X1 = CH2, O) and in AcOH to give imidazolinones I (R = Cl, H, R1 = 4-NO2; X = NC6H4Me-4). II reacted with R3NHNH2 (R3 = H, Ph) in EtOH to give hydrazides III (R2 = NHR3) and with PhNHNH2 in AcOH to give triazines V (R1 = H, 3-Cl) (1 tautomer shown). NH2OH.HCl reacted with II (R = Cl, R1 = H, 3-Cl; R = NO2, R1 = 2-Br, 4-NMe2) to give imidazolones I (X = NOH, VI) which reacted with PhNHNH2 to give V. Tetrazoles VII (R's as for VI), were prepared from II and NaN3.
IT 90125-21-6P 90125-22-7P 90125-23-8P 90125-24-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 90125-21-6 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(4-chlorophenyl)-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

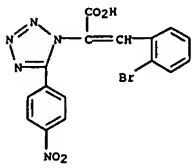


RN 90125-22-7 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(4-chlorophenyl)-α-[(3-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)

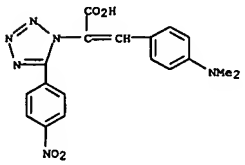
L4 ANSWER 171 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



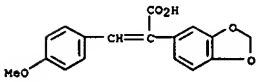
RN 90125-23-8 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[(2-bromophenyl)methylene]-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



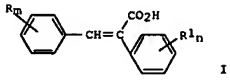
RN 90125-24-9 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[[4-(dimethylamino)phenyl]methylene]-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



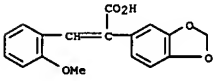
L4 ANSWER 172 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 172 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:612230 CAPLUS
DOCUMENT NUMBER: 99:212230
TITLE: Studies on the nonsteroidal antifertility agents. II. Synthesis and antifertility activity of some p-coumaric acid derivatives
AUTHOR(S): Zhu, Chongquang; Zhang, Yihua; Cao, Guangkun; Peng, Sixun; Wang, Wenhua; Zheng, Jinhai
CORPORATE SOURCE: Div. Med. Chem., Nanjing Coll. Pharm., Nanjing, Peop. Rep. China
SOURCE: Nanjing Yaoxueyuan Xuebao (1982), (3), 50-6
CODEN: NYXUDF; ISSN: 0254-5055
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

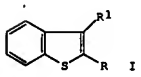


AB Twenty-four coumaric acid derivs. (I; R = alkoxy, HO, Cl, OCH2O; R1 = H, MeO, OCH2O; m, n = 1, 2; R1n = benzo) were prepared Some I were effective in terminating early pregnancy at 50 mg/kg in mice.
IT 87751-89-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antifertility activity of)
RN 87751-89-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

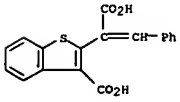


IT 87751-90-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87751-90-4 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 173 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:594748 CAPLUS
DOCUMENT NUMBER: 99:194748
TITLE: Synthesis of pyrano/pyridobenzothiophene derivatives. Part-I
AUTHOR(S): Chatterjea, J. N.; Sahai, Radhika P.
CORPORATE SOURCE: Dep. Chem., Patna Univ., Patna, 800 005, India
SOURCE: Journal of the Indian Chemical Society (1982), 59(11-12), 1372-4
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:194748
GI



AB The benzothiophenedicarboxylate I (R = R1 = CO2Me) with prepared by treating 2,3-benzothiophenedione with ClCH2CO2H. I (R = R1 = CO2Me) was converted to I (R = CO2H, H, CH2CO2Me, CH2OH, CHO, R1 = CO2Me; R = H, CH2CO2H, R1 = CO2H). I [RR1 = CH2C(O)OC(O), C(:CHPh)C(O)OC(O), CH:C(CO2H)OC(O), CH:C(CO2H)NHC(O)] were also prepared
IT 87807-54-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)
RN 87807-54-3 CAPLUS
CN Benzo[b]thiophene-2-acetic acid, 3-carboxy-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



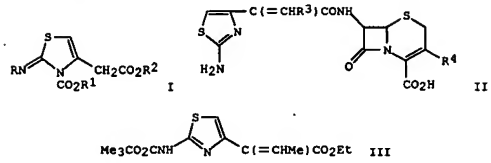
L4 ANSWER 174 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:522170 CAPLUS
DOCUMENT NUMBER: 99:122170
TITLE: Intermediates useful in the preparation of cephalosporins
INVENTOR(S): Kinast, Guenther
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 45 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3145727	A1	19830526	DE 1981-3145727	19811119
US 4500716	A	19850219	US 1982-438189	19821101
EP 81674	A1	19830622	EP 1982-110254	19821106
EP 81674	B1	19870708		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 28196	T	19870715	AT 1982-110254	19821106
JP 58092672	A	19830602	JP 1982-199850	19821116
JP 02042830	B	19900926		
CA 1212949	A1	19861021	CA 1982-415708	19821117
DK 8205151	A	19830520	DK 1982-5151	19821118
ZA 8208494	A	19831026	ZA 1982-8494	19821118
HU 27881	A2	19831128	HU 1982-3710	19821118
HU 187816	B	19860228		
ES 517514	A1	19831001	ES 1982-517514	19821119
CA 1238911	A2	19880705	CA 1986-505254	19860326
CA 1240985	A2	19880823	CA 1987-541405	19870706
CA 1247109	A2	19881220	CA 1987-541321	19870706
JP 02288870	A	19901128	JP 1990-109001	19900426
JP 03068027	B	19911025		

PRIORITY APPLN. INFO.: DE 1981-3145727 A 19811119
EP 1982-110254 A 19821106
CA 1982-415708 A3 19821117
CA 1986-505254 A3 19860326

OTHER SOURCE(S): MARPAT 99:122170
GI

L4 ANSWER 174 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

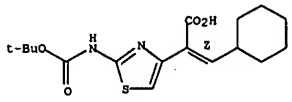


I II

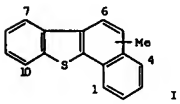
III

AB Thiazolines I [R = protective group; R1, R2 = (un)substituted alkyl, cycloalkyl, aryl, heterocyclic], useful as intermediates for cephalosporins II [R3 = (un)substituted alkyl, cycloalkyl, aryl, heterocyclic; R4 = appropriate substituent], were prepared Thus Et 2-amino-4-thiazolylacetate was treated with (Me3CO2C)2O to give I (R = Me3CO2C, R1 = CMe3, R2 = Et) which was treated with MeCHO to give III. Saponification of III to the acid, successive reaction with MeSO2Cl and 7-aminocephalosporanic acid, and deblocking gave II (R3 = Me, R4 = CH2OAc).
IT 86978-31-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of aminocephems by)
RN 86978-31-6 CAPLUS
CN 4-Thiazoleacetic acid, α-(cyclohexylmethylene)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



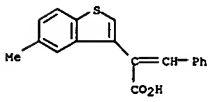
L4 ANSWER 175 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:4452 CAPLUS
DOCUMENT NUMBER: 98:4452
TITLE: The synthesis of the monomethyl isomers of benzo[b]naphtho[2,1-d]thiophene
AUTHOR(S): Tominaga, Yoshinori; Pratap, Ram; Castle, Raymond N.; Lee, Milton L.
CORPORATE SOURCE: Dep. Chem., Univ. South Florida, Tampa, FL, 33620, USA
SOURCE: Journal of Heterocyclic Chemistry (1982), 19(4), 859-63
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



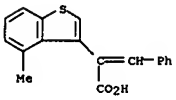
I

AB All isomers of the monomethylbenzo[b]naphtho[2,1-d]thiophenes (I) were prepared by photocyclization of 3-styrylbenzo[b]thiophenes. The 1-, 3-, 4-, and 5-methylbenzo[b]naphtho[2,1-d]thiophenes were prepared by irradiation of the corresponding methylated 3-styrylbenzo[b]thiophenes which were prepared by the Wadsworth-Emmons reaction of di-Et benzo[b]thenylphosphonate with tolualdehydes and PhCOMe. The 7-, 8-, 9- and 10-methylbenzo[b]naphtho[2,1-d]thiophenes were synthesized by decarboxylation of 7-, 8-, 9- and 10-methylbenzo[b]naphtho[2,1-d]thiophene-6-carboxylic acid with Cu in quinoline. These carboxylic acids were prepared by photocyclization of the corresponding 2-(benzo[b]thiophen-3-yl)-3-phenylpropenoic acids which were prepared by the condensation of the methylated benzo[b]thiophene-3-ylacetic acids with PhCHO in the presence of Et3N-Ac2O.
IT 83821-47-0P 83821-48-1P 83821-49-2P 83821-50-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photochem. cyclization of)
RN 83821-47-0 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, 5-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

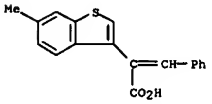
L4 ANSWER 175 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



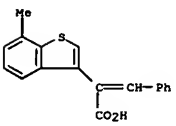
RN 83821-48-1 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, 4-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



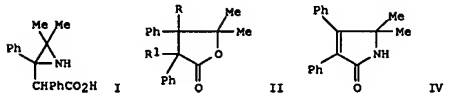
RN 83821-49-2 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, 6-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 83821-50-5 CAPLUS
CN Benzo[b]thiophene-3-acetic acid, 7-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



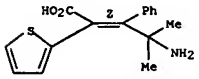
L4 ANSWER 176 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:562719 CAPLUS
DOCUMENT NUMBER: 97:162719
TITLE: Addition of reactive dimetallic ambidents to the azirine double bond
AUTHOR(S): Blagoev, B.; Novkova, S.
CORPORATE SOURCE: Inst. Chim. Org., Sofia, 1113, Bulg.
SOURCE: Tetrahedron (1982), 38(11), 1609-13
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 97:162719
GI



I II IV

AB Ivanov Mg reagents, prepared by reaction of arylacetic acids with Me2CHMgCl,
added to 3,3-dimethyl-2-phenylazirine (Ia) to give β-aziridino acids. The latter readily underwent intramol. cycloaddn. to 4-amino lactones, which on warming lost NH3 to give butenolides. E.g., reaction of PhCH2CO2H with Me2CHMgCl in refluxing MeOH for 2.5 h, addition of Ia, and refluxing for 6 h gave 65% aziridine I. I in EtOH at room temperature in <24 h
gave 50% lactone II (R = NH2, R1 = H), which on refluxing in H2O for 2 h gave >90% II (RR1 = bond). Reaction of the arylacetic acids with sodium naphthalene (III) gave pyrrolidinones and E-γ-aminocrotonic acids. E.g., reaction of PhCH2CO2H with III in THF at 50° for 2 h gave 25% (E)-HO2CCPh:CPhCMe2NH2 and 41% pyrrolidinone IV.
IT 83253-83-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 83253-83-2 CAPLUS
CN 2-Thiopheneacetic acid, α-(2-amino-2-methyl-1-phenylpropylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 176 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

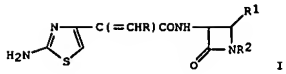
L4 ANSWER 177 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:527391 CAPLUS
DOCUMENT NUMBER: 97:127391
TITLE: β-Lactam antibiotics and compositions containing them
INVENTOR(S): Boberg, Michael; Metzger, Karl Georg
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Eur. Pat. Appl., 110 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 49448	A2	19820414	EP 1981-107679	19810928
EP 49448	A3	19830511		
EP 49448	B1	19880824		
R: AT, BE, CH, DE, FR, GB, IT, NL, SE				
DE 3037997	A1	19820513	DE 1980-3037997	19801008
US 4416880	A	19831122	US 1981-304280	19810921
IL 63959	A	19850731	IL 1981-63959	19810928
IL 72435	A	19850731	IL 1981-72435	19810928
AT 36714	T	19880915	AT 1981-107679	19810928
FI 8103089	A	19820409	FI 1981-3089	19811006
FI 75825	B	19880429		
FI 75825	C	19880808		
JP 57093982	A	19820611	JP 1981-158247	19811006
JP 05037995	B	19930607		
CA 1178946	A1	19841204	CA 1981-387441	19811006
DK 8104445	A	19820409	DK 1981-4445	19811007
DK 165924	B	19930208		
DK 165924	C	19930628		
ZA 8106932	A	19820929	ZA 1981-6932	19811007
AU 8176133	A	19820422	AU 1981-76133	19811008
AU 554294	B2	19860814		
ES 506115	A1	19820816	ES 1981-506115	19811008
HU 26732	A2	19830928	HU 1981-2910	19811008
HU 186429	B	19850729		
JP 61093173	A	19860512	JP 1985-237801	19851025
JP 63037107	B	19880722		
JP 61106579	A	19860524	JP 1985-237800	19851025
JP 02209877	A	19900821	JP 1989-150323	19890613
JP 06062631	B	19940817		

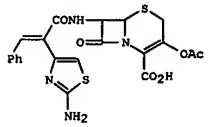
PRIORITY APPLN. INFO.: DE 1980-3037997 A 19801008
EP 1981-107679 A 19810928
IL 1981-63959 A 19810928

OTHER SOURCE(S): MARPAT 97:127391
GI

L4 ANSWER 177 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



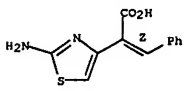
I



II

AB β-Lactams I [R = H, (un)substituted alkyl, Ph, polycyclic aromatic, heterocyclic; R1R2 = OCH2CR3:CCO2H, SCH2CR3:CCO2H, SCMe2CHCO2H; R3 = organic]
were prepared PhCH:C(COMe)CO2Et was brominated and cyclized with thiourea
to give Et 2-(2-amino-4-thiazolyl)-3-phenylpropenoate which was saponified
and used to acylate 7- aminocephalosporanic acid to give II.
IT 82617-91-2P 82618-07-3P 82618-08-4P
82618-35-7P 82618-46-0P 82619-20-3P
82619-24-7P 82619-29-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of aminocephems by)
RN 82617-91-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(phenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

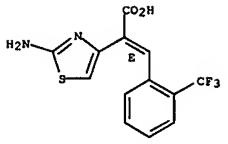
Double bond geometry as shown.



RN 82618-07-3 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[[2-(trifluoromethyl)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

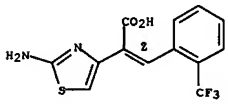
Double bond geometry as shown.

L4 ANSWER 177 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



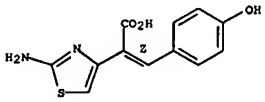
RN 82618-08-4 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[[2-(trifluoromethyl)phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 82618-35-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

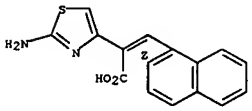
Double bond geometry as shown.



RN 82618-46-0 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(1-naphthalenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

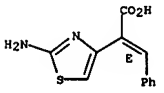
Double bond geometry as shown.

L4 ANSWER 177 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



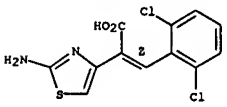
RN 82619-20-3 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 82619-24-7 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(2,6-dichlorophenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

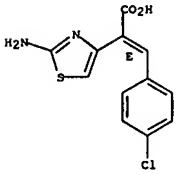
Double bond geometry as shown.



RN 82619-29-2 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(4-chlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

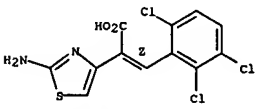
Double bond geometry as shown.

L4 ANSWER 177 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



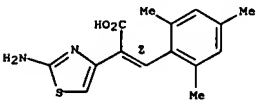
IT 82618-16-4P 82619-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phosphorus pentachloride)
RN 82618-16-4 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(2,3,6-trichlorophenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 82619-50-9 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(2,4,6-trimethylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

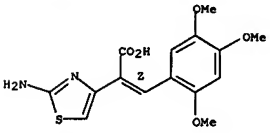
Double bond geometry as shown.



IT 82618-31-3P 82623-34-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82618-31-3 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(2,4,5-trimethoxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

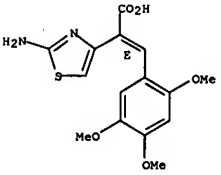
Double bond geometry as shown.

L4 ANSWER 177 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

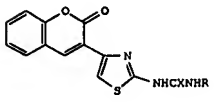


RN 82623-34-5 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(2,4,5-trimethoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

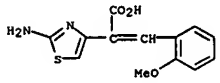


L4 ANSWER 178 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:52221 CAPLUS
DOCUMENT NUMBER: 96:52221
TITLE: Some derivatives of coumarinylthiazolylurea and thiourea. I
AUTHOR(S): Gursoy, Aysel; Gokcek, Duygu
CORPORATE SOURCE: Eczacilik Fak., Istanbul Univ., Istanbul, Turk.
SOURCE: Doga Bilim Dergisi, Seri C: Tip (1981), 5(1), 27-38
CODEN: DSTIDB; ISSN: 0254-2331
DOCUMENT TYPE: Journal
LANGUAGE: Turkish
GI



I

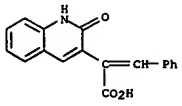
AB Ureas I (X = O, R = Ph, 1-naphthyl, coumarinylthiazolyl; X = S, R = allyl, Bu, PhCH2CH2, 4-ClC6H4, 4-BrC6H4) were obtained in 34.8-82.6% yield by treating the amines with RNCO, COCl2, RNCS.
IT 80556-88-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 80556-88-3 CAPLUS
CN 4-Thiazoleacetic acid, 2-amino-α-[(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 179 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:35046 CAPLUS
DOCUMENT NUMBER: 96:35046
TITLE: Synthesis of benzo[k]phenanthridines: another new approach
AUTHOR(S): Arisvaran, V.; Ramesh, M.; Rajendran, S. P.; Shanmugam, P.
CORPORATE SOURCE: Post-Grad. Cent., Madras Univ., Coimbatore, 641 041, India
SOURCE: Synthesis (1981), (10), 821-3
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:35046
GI

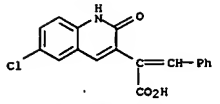
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Refluxing quinolines I (R = H, Cl, Me) with PHCHO, HOAc and Ac2O gave II. Treating II with aqueous NaOH followed by acidification gave III (R1 = CO2H), decarboxylation of which gave III (R1 = H). Irradiation of III (R1 = H) gave IV (R2 = H), chlorination of which gave V (R2 = H). Irradiation of II in MeOH gave IV (R2 = CO2Me), chlorination of which gave V (R2 = CO2Me).
IT 80356-55-4P 80356-56-5P 80356-57-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)
RN 80356-55-4 CAPLUS
CN 3-Quinolineacetic acid, 1,2-dihydro-2-oxo-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

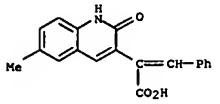


RN 80356-56-5 CAPLUS
CN 3-Quinolineacetic acid, 6-chloro-1,2-dihydro-2-oxo-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

L4 ANSWER 179 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

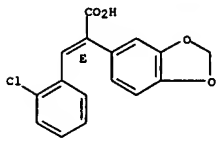


RN 80356-57-6 CAPLUS
CN 3-Quinolineacetic acid, 1,2-dihydro-6-methyl-2-oxo-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

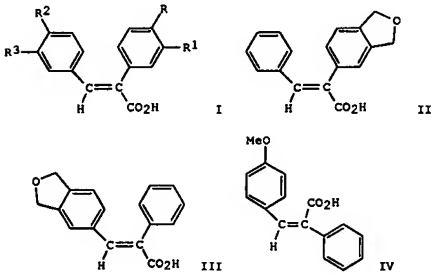


L4 ANSWER 180 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:461683 CAPLUS
DOCUMENT NUMBER: 95:61683
TITLE: Reactions of halogenated α-phenylcinnamic acids with potassium amide in liquid ammonia. Part I. Reactions of cis- and trans-2-chloro-α-phenylcinnamic acids
AUTHOR(S): Kessar, S. V.; Nadir, U. K.; Gupta, Y. P.; Pahwa, P. S.; Singh, Paramjit
CORPORATE SOURCE: Dep. Chem., Panjab Univ., Chandigarh, 160 014, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1981), 20B(1), 1-3
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:61683
AB Reaction of trans- and cis-2-chloro-α-phenylcinnamic acids with KNH2 in NH3 (l) gave phenanthrene-9-carboxylic acids and 3-phenylcarbostyrils. Under similar conditions 3-chloro-α-phenylcinnamic acids gave 3-phenylcoumarins.
IT 78423-43-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with potassium amide in liquid ammonia)
RN 78423-43-5 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(2-chlorophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



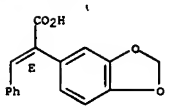
L4 ANSWER 181 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:406177 CAPLUS
DOCUMENT NUMBER: 95:6177
TITLE: Isomerization of α-phenylcinnamic acids with potassium amide in liquid ammonia
AUTHOR(S): Kessar, S. V.; Nadir, U. K.; Narula, Suchita; Kumar, Pawan; Mohammad, Taj
CORPORATE SOURCE: Dep. Chem., Panjab Univ., Chandigarh, 160 014, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1981), 20B(1), 4-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Isomerization of I (R, R1, R2, R3 given: H, H, H, H; MeO, H, H, H; H, H, MeO, H; NO2, H, H, H), II, and III with KNH2 yields the corresponding geometric isomer (e.g. IV) via a radical ion or charge-transfer complex intermediate.
IT 77955-67-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(isomerization of, mechanism of)
RN 77955-67-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

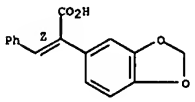
Double bond geometry as shown.

L4 ANSWER 181 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

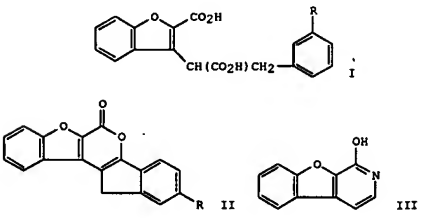


IT 77955-68-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 77955-68-1 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-(phenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

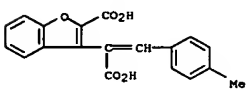
Double bond geometry as shown.



L4 ANSWER 182 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:139660 CAPLUS
DOCUMENT NUMBER: 94:139660
TITLE: Syntheses of furano compounds. Part XLV. Syntheses of 1-oxo-1H-benzo[b]furo[4,3-d]indeno[2',1':5,6]pyrans and nitrogen analogs
AUTHOR(S): Chatterjea, J. N.; Sahai, Radhika Pati
CORPORATE SOURCE: Dep. Chem., Patna Univ., Patna, 800 005, India
SOURCE: Journal of the Indian Chemical Society (1980), 57(12), 1163-5
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:139660
GI

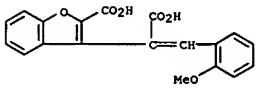


AB Cyclizing benzofuranacetic acids I (R = H, OMe) gave benzofuroindenopyrans
II, ammonolysis of which gave III.
IT 77116-89-3P 77116-92-8P 77116-95-1P
77117-04-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 77116-89-3 CAPLUS
CN 3-Benzofuranacetic acid, 2-carboxy-α-[(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)

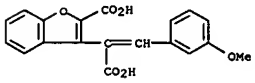


RN 77116-92-8 CAPLUS
CN 3-Benzofuranacetic acid, 2-carboxy-α-[(2-methoxyphenyl)methylene]-

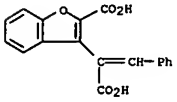
L4 ANSWER 182 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



RN 77116-95-1 CAPLUS
CN 3-Benzofuranacetic acid, 2-carboxy-α-[(3-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



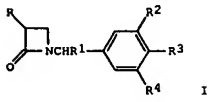
RN 77117-04-5 CAPLUS
CN 3-Benzofuranacetic acid, 2-carboxy-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



L4 ANSWER 183 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:65461 CAPLUS
DOCUMENT NUMBER: 94:65461
TITLE: 4-Unsubstituted azetidinone derivatives
INVENTOR(S): Hashimoto, Masashi; Hemmi, Keiji; Kamiya, Takashi; Komori, Tadaaki; Nakaguti, Osamu; Saito, Yoshihisa; Shiokawa, Youichi; Takasugi, Hisshi; Takaya, Takao; Teraji, Tsutomu
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: U.S., 130 pp. Cont.-in-part of U.S. Ser. No. 694,891, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4207234	A	19800610	US 1977-858375	19771207
US 4472300	A	19840918	US 1980-130205	19800313
PRIORITY APPLN. INFO.:			US 1975-593668 A2	19750707
			US 1976-694891 A2	19760610
			US 1977-858375 A3	19771207

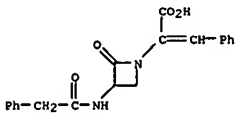
OTHER SOURCE(S): CASREACT 94:65461; MARPAT 94:65461
GI



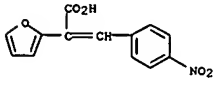
I

AB Lactacillanic acids and analogs I (R = NH2, acylamino, benzenesulfonamido; R1 = CO2H, pharmaceutically acceptable salt or ester derivative of CO2H; R2 = H, NH2, NO2, halo, alkoxy, alkylthio; R3 = H, OH, alkyl, alkylthio, OCH2Ph; R4 = H, Halo, alkoxy, alkylthio), which showed bactericidal activity, were prepared Thus, 3-aminolactacillanic acid reacted with PhCH2COCl in water-Me2CO containing NaHCO3 to yield I (R = PhCH2CONH, R1 = CO2H, R3 = OH, R2 = R4 = H).
IT 64026-84-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64026-84-2 CAPLUS
CN 1-Azetidineacetic acid, 2-oxo-3-[(phenylacetyl)amino]-α-

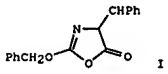
L4 ANSWER 183 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(phenylmethylene)- (9CI) (CA INDEX NAME)



L4 ANSWER 184 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:617105 CAPLUS
DOCUMENT NUMBER: 93:217105
TITLE: Studies on enzymic cis-trans isomerization of nitrothiophene and nitrobenzene derivatives
AUTHOR(S): Tatsumi, Kiyoshi; Koga, Nobuyuki; Yoshimura, Hidetoshi
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Journal of Pharmacobio-Dynamics (1980), 3(7), 339-44
CODEN: JOPHDQ; ISSN: 0386-846X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The enzymic cis-trans isomerization of nitrothiophene and nitrobenzene derivs. was comparatively investigated by using the geometrical isomers of 3-(5-nitro-2-thienyl)-2-(2-furyl)acrylamide and 3-(4-nitrophenyl)-2-(2-furyl)-acrylamide. The nitrothiophene derivative was mainly isomerized from the cis to the trans form by milk xanthine oxidase or rat liver microsomes supplemented with an electron donor. In the case of the nitrobenzene derivative, however, such enzymic cis-trans isomerization was not observed in these enzyme systems.
IT 75499-53-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with ammonium hydroxide)
RN 75499-53-5 CAPLUS
CN 2-Furanacetic acid, α-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

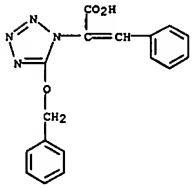


L4 ANSWER 185 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:514367 CAPLUS
DOCUMENT NUMBER: 93:114367
TITLE: The preparation and reactions of 2-benzyloxy-4-benzylideneoxazol-5-one
AUTHOR(S): Jones, John H.; Witty, Michael J.
CORPORATE SOURCE: Dyson Perrins Lab., Univ. Oxford, Oxford, OX1 3QY, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1980), (4), 858-64
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The title compound(Z-I) was prepared (48%) by treatment of N-(benzyloxycarbonyl)-threo-β-phenylserine with PC15 at low temperature, followed by addition of Et3N; the corresponding erythro isomer also gave Z-I, but in lower yield (27%). The reactivity at C-5 of Z-I towards nucleophiles is high compared with that of the corresponding 2-Ph compound (II), and nucleophilic reagents attack Z-I exclusively at this position in contrast to the behavior of II. Thus, Z-I underwent regiospecific ring cleavage with a variety of nucleophilic reagents.
IT 74805-44-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74805-44-0 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(phenylmethoxy)-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



L4 ANSWER 185 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 186 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:87240 CAPLUS
DOCUMENT NUMBER: 90:87240
TITLE: Azetidinone derivatives
INVENTOR(S): Kamiya, Takashi; Saito, Norihisa; Hashimoto, Masashi; Teraji, Tsutomu; Takaya, Takao; Komori, Tadaaki; Nakaguchi, Osamu; Oku, Teruo; Shiokawa, Yoichi; et al.
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

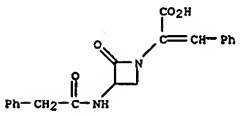
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53095957	A	19780822	JP 1977-150275	19771213
SE 7614001	A	19770617	SE 1976-14001	19761213
FR 2335212	A2	19770715	FR 1976-37763.	19761215
PRIORITY APPLN. INFO.:			SE 1976-14001 A	19761213
			FR 1976-37763 A	19761215
			JP 1975-150909 A	19751216
			JP 1975-150910 A	19751216
			JP 1975-150911 A	19751216
			JP 1975-150912 A	19751216
			JP 1975-158511 A	19751230
			JP 1976-190 A	19760101
			GB 1976-21507 A	19760525

GI

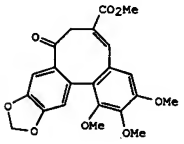
I

AB Forty azetidinone derivs. I [R = 4-(3-phthalimidopropoxy)phenylglyoxyloyla mino, 2-[2-(2,2,2-trifluoroacetamido)-4-thiazolyl]-2-methoxyiminoacetamido, etc.; R1 = 1-carboxy-2-methyl-1-propenyl, α-carboxy-4-phenylacetoxybenzyl, etc.] were prepared Min. inhibitory concns. of some of I against Escherichia coli, Pseudomonas aeruginosa, and

L4 ANSWER 186 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Proteus vulgaris were 2-18 μg/mL. Thus, stirring 236 mg 2-(4-hydroxyphenyl)-2-(3-amino-2-oxo-1-azetidinyl)acetic acid with 1 g N,O-bis(trimethylsilyl)acetamide in CH2Cl2 5 h at room temp. and stirring with 2-methoxyimino-2-[2-(2,2,2,-trifluoroacetamido)-4-thiazolyl]acetyl chloride 2.5 h at -30°, 2 h at 0-5°, and overnight at room temp. gave 280 mg 2-(4-hydroxyphenyl)-2-[3-[2-methoxyimino-2-[2-(2,2,2-trifluoroacetamido)-4-thiazolyl]acetamido]-2-oxo-1-azetidinyl]acetic acid.
IT 64026-84-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64026-84-2 CAPLUS
CN 1-Azetidineacetic acid, 2-oxo-3-[(phenylacetyl)amino]-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

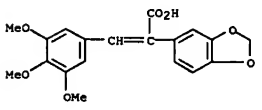


L4 ANSWER 187 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:579893 CAPLUS
DOCUMENT NUMBER: 89:179893
TITLE: Dibenzocyclooctadiene antileukemic lignan synthesis. (±)-Steganone
AUTHOR(S): Krow, Grant R.; Damodaran, Kalyani M.; Michener, Edward; Wolf, Robert; Guare, James
CORPORATE SOURCE: Dep. Chem., Temple Univ., Philadelphia, PA, USA
SOURCE: Journal of Organic Chemistry (1978), 43(20), 3950-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A new route to the unsatd. oxo ester I, an intermediate in the Raphael synthesis of steganone and its companion antileukemic lignans steganacin and steganangin was described. Key reactions utilized in the synthetic sequence were photochem. ring closure of a stilbenecarboxylic acid to a phenanthrene, the trimethylsilyl azide modification of the Curtius rearrangement of carboxylic acids, and a two-carbon ring expansion of a 9-phenanthrylamine with MeO2CC.tplbond.CCO2Me.
IT 60848-05-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. cyclization of, phentherine derivative from)
RN 60848-05-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(3,4,5-trimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

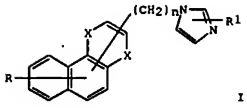


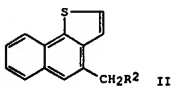
L4 ANSWER 188 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:509490 CAPLUS
DOCUMENT NUMBER: 89:109490
TITLE: Imidazole derivatives
INVENTOR(S): Blattner, Hans; Storni, Angelo
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2753054	A1	19780608	DE 1977-2753054	19771128
GB 1590648	A	19810603	GB 1977-48953	19771124
US 4171366	A	19791016	US 1977-854935	19771125
FI 7703593	A	19780602	FI 1977-3593	19771128
FR 2372829	A1	19780630	FR 1977-35727	19771128
FR 2372829	B1	19820604		
CA 1097351	A1	19810310	CA 1977-291993	19771129
BE 861337	A1	19780530	BE 1977-183038	19771130
DK 7705319	A	19780602	DK 1977-5319	19771130
NO 7704101	A	19780602	NO 1977-4101	19771130
NO 146600	B	19820726		
NO 146600	C	19821103		
SE 7713574	A	19780602	SE 1977-13574	19771130
NL 7713241	A	19780605	NL 1977-13241	19771130
ES 464611	A1	19780901	ES 1977-464611	19771130
ZA 7707129	A	19780927	ZA 1977-7129	19771130
AU 7731087	A	19790607	AU 1977-31087	19771130
AU 517512	B2	19810806		
AT 7708571	A	19800815	AT 1977-8571	19771130
AT 361469	B	19810310		
JP 53068776	A	19780619	JP 1977-143343	19771201
AT 8001366	A	19800815	AT 1980-1366	19800312
AT 361472	B	19810310		

PRIORITY APPLN. INFO.: LU 1976-76303 A 19761201
AT 1977-8571 A 19771130

GI


I


II

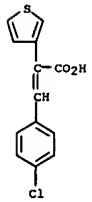
L4 ANSWER 188 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB The imidazole derivs. I (R = R1 = H, halogen, alkyl, etc.; one of X = S, or CH:CH, the other is a single bond; n = 1-4) and their salts were prepared for use as antidepressants at 0.10-10 mk/kg/day. Thus, Grignard reaction of MeI with benzo[f]thieno[2,3-b]thiepin-4(5H)-one, followed by dehydration with H2SO4 gave 4-methylbenzo[f]thieno[2,3-b]thiepin, which was refluxed with KOH in HOCH2CH2OH to give II (R2 = H). This was brominated with N-bromosuccinimide, followed by reaction with imidazole to give II (R2 = 1H-imidazol-1-yl).

IT 67523-13-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 67523-13-1 CAPLUS

CN 3-Thiopheneacetic acid, α-[(4-chlorophenyl)methylene]- (9CI) (CA INDEX NAME)

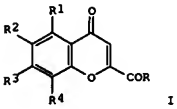


L4 ANSWER 189 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:443115 CAPLUS
DOCUMENT NUMBER: 89:43115
TITLE: Benzopyran derivatives
PATENT ASSIGNEE(S): Fisons Ltd., UK
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52142073	A	19771126	JP 1977-56051	19770517
FI 7701545	A	19771120	FI 1977-1545	19770516
NO 7701722	A	19771122	NO 1977-1722	19770516
SE 7705849	A	19771120	SE 1977-5849	19770517
ES 458912	A1	19780716	ES 1977-458912	19770518

PRIORITY APPLN. INFO.: GB 1976-20571 A 19760519
GB 1977-13285 A 19770330

GI


I

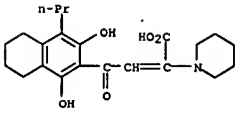
AB The benzopyranones I [R = OH, NH2; R1 = H, OH; R2-R4 = alkyl or R2R3 = (CH2)4] were prepared by cyclization of 3-aroylacrylic acids. Thus, a solution of 2-amino-3-(3,5-di-tert-butyl-2-hydroxybenzoyl)acrylic acid in EtOH saturated with HCl at room temperature gave I (R = NH2, R1 = R3 = H, R2 = R4 = CMe3). I [R = R1 = OH, R2 = R4 = Et, R3 = H; R = R1 = OH, R2R3 = (CH2)4, R4 = Pr] were prepared similarly.

IT 66982-35-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, benzopyran derivative from)

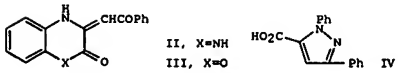
RN 66982-35-2 CAPLUS

CN 1-Piperidineacetic acid, α-[2-oxo-2-(5,6,7,8-tetrahydro-1,3-dihydroxy-4-propyl-2-naphthalenyl)ethylidene]- (9CI) (CA INDEX NAME)

L4 ANSWER 189 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

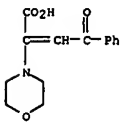


L4 ANSWER 190 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:62102 CAPLUS
DOCUMENT NUMBER: 88:62102
TITLE: Benzoylpropiolic acid in a nucleophilic addition reaction
AUTHOR(S): Bol'shedvorskaya, R. L.; Pavlova, G. A.; Alekseeva, N. V.; Vereshchagin, L. I.
CORPORATE SOURCE: Inst. Nefte- Uglekhim. Sint., Irkutsk, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1977), 13(11), 2317-20
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



II, X=NH
III, X=O
IV

AB PhCOC.tplbond.CO2H (I) underwent addition reactions with amines RR1NH (R = H, R1 = Ph, p-tolyl, 2-naphthyl; R = Et, R1 = Ph; or RR1N = morpholino) in absolute ether to give <80.3% PhCOCH:C(NRR1)CO2H. The reaction of I with aliphatic amines and OH-containing compds. is accompanied by hydrolysis of the adducts to give PhCOCH2COCO2H. I with C6H4(NH2)2-o, p-HOC6H4NH2, or PhNHNH2 gave the cyclic adducts II, III, and IV, resp.
IT 65387-44-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 65387-44-2 CAPLUS
CN 4-Morpholineacetic acid, α-(2-oxo-2-phenylethylidene)- (9CI) (CA INDEX NAME)



L4 ANSWER 191 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:551998 CAPLUS
DOCUMENT NUMBER: 87:151998
TITLE: Azetidinone derivatives
INVENTOR(S): Kamiya, Takashi; Saito, Yoshihisa; Hoshimoto, Masashi; Teraji, Tsutomu; Takaya, Takao; Komori, Tadaaki; Nakaguti, Osamu; Oku, Teruo; Shiokawa, Youichi; et al.
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Ger. Offen., 110 pp. Addn. to Ger. Offen. 2,529,941.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2657079	A1	19770707	DE 1976-2657079	19761216
JP 52073854	A	19770621	JP 1975-150909	19751216
JP 52073855	A	19770621	JP 1975-150910	19751216
JP 52073856	A	19770621	JP 1975-150911	19751216
JP 52073857	A	19770621	JP 1975-150912	19751216
JP 52083451	A	19770712	JP 1975-158511	19751230
JP 52083541	A	19770712	JP 1976-190	19760101
JP 60042237	B	19850920		
BE 849445	A4	19770615	BE 1976-173295	19761215
NL 7613973	A	19770620	NL 1976-13973	19761216
AT 7902057	A	19820715	AT 1979-2057	19790319
AT 370092	B	19830225		
AT 7902056	A	19821015	AT 1979-2056	19790319
AT 371108	B	19830610		
ES 479039	A1	19790701	ES 1979-479039	19790329
US 4304718	A	19811208	US 1979-71280	19790830
US 4472309	A	19840918	US 1981-296114	19810825
CH 642350	A5	19840413	CH 1982-3245	19820526
US 4576753	A	19860318	US 1984-629216	19840709

PRIORITY APPLN. INFO.:
JP 1975-150909 A 19751216
JP 1975-150910 A 19751216
JP 1975-150911 A 19751216
JP 1975-150912 A 19751216
JP 1975-158511 A 19751230
JP 1976-190 A 19760101
GB 1976-21507 A 19760525
GB 1975-40893 A 19751006
GB 1976-94 A 19760102

L4 ANSWER 191 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

GB 1976-242	A	19760105
GB 1976-25746	A	19760621
AT 1976-7392	A	19761005
CH 1976-12645	A	19761006
US 1976-730012	A	19761006
US 1979-71280	A3	19790830
US 1981-296114	A3	19810825

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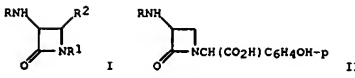
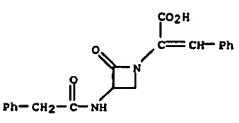


I II

AB About 140 azetidinone derivs. I [R=H, acyl; R1=H, CHR3R4 (where R3 = substituted phenyl, C10H7, aralkyl, arylthioalkyl, etc.; R4=CO2H, carboxyalkyl or derivative), CR5:CR6R7 (where R5 = CO2H or derivative; R6 = H, alkyl; R7 = alkyl, heterocyclylthioalkyl, arylthio); R2 = H, HOCH2, aryl, aralkenyl] were prepared for use as bactericides. Thus, II (R=H) was stirred with CH2Cl2, N,O-bis(trimethylsilyl)acetamide, and DMF, followed by the addition of Et3N and PhCOCOCl to give II (R=PhCOCO). I were tested on E. coli, S. aureus, etc., and the results were tabulated.
IT 64026-84-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64026-84-2 CAPLUS
CN 1-Azetidineacetic acid, 2-oxo-3-[(phenylacetyl)amino]-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



L4 ANSWER 192 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:502148 CAPLUS
DOCUMENT NUMBER: 87:102148
TITLE: 2-Azetidinone compounds
INVENTOR(S): Kamiya, Takashi; Hashimoto, Masashi; Nakaguti, Osamu; Oku, Teruo; Nakai, Yoshiharu; Takeno, Hidekazu
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Ger. Offen., 182 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

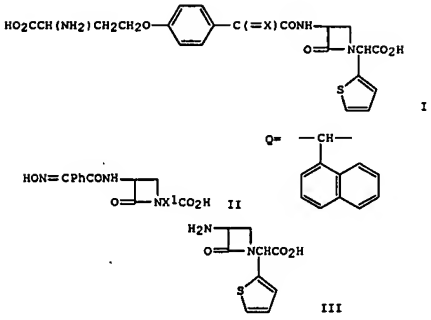
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2645085	A1	19770414	DE 1976-2645085	19761006
GB 1570278	A	19800625	GB 1975-40893	19751006
AU 516665	B2	19810618	AU 1976-18405	19761001
BE 846934	A1	19770404	BE 1976-171233	19761004
FR 2326920	A1	19770506	FR 1976-29942	19761005
FR 2326920	B1	19820827		
DK 7604510	A	19770407	DK 1976-4510	19761006
FI 7602843	A	19770407	FI 1976-2843	19761006
SE 7611103	A	19770407	SE 1976-11103	19761006
SE 438853	B	19850513		
NL 7611027	A	19770412	NL 1976-11027	19761006
NO 7603402	A	19770412	NO 1976-3402	19761006
JP 52065263	A	19770530	JP 1976-120736	19761006
JP 61003784	B	19860204		
ZA 7605984	A	19780530	ZA 1976-5984	19761006
US 4181800	A	19800101	US 1976-730012	19761006
CH 630073	A5	19820528	CH 1976-12645	19761006
FR 2408593	A1	19790608	FR 1977-18241	19770614
FR 2408593	B1	19820709		
FR 2384747	A1	19781020	FR 1978-7885	19780317
FR 2384747	B1	19820813		
ES 471792	A1	19791016	ES 1978-471792	19780717
AT 7902057	A	19820715	AT 1979-2057	19790319
AT 370092	B	19830225		
AT 7902056	A	19821015	AT 1979-2056	19790319
AT 371108	B	19830610		
ES 479039	A1	19790701	ES 1979-479039	19790329
US 4304718	A	19811208	US 1979-71280	19790830
SE 8103640	A	19810610	SE 1981-3640	19810610
US 4472309	A	19840918	US 1981-296114	19810825
CH 642350	A5	19840413	CH 1982-3245	19820526
US 4576753	A	19860318	US 1984-629216	19840709
JP 61010552	A	19860118	JP 1984-280812	19841224
JP 01006190	B	19890202		

PRIORITY APPLN. INFO.:
GB 1975-40893 A 19751006
GB 1976-94 A 19760102
GB 1976-242 A 19760105
GB 1976-21507 A 19760525
GB 1976-25746 A 19760621

L4 ANSWER 192 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AT 1976-7392	A	19761005
CH 1976-12645	A	19761006
US 1976-730012	A	19761006
US 1979-71280	A3	19790830
US 1981-296114	A3	19810825

OTHER SOURCE(S): MARPAT 87:102148
GI



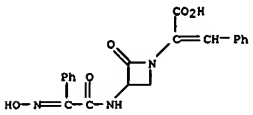
I

II

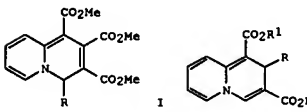
III

AB Azetidinones, such as I (X = O, NOH) and II (X1 = Q, C:CHPh) were prepared
Thus I (X = O) was obtained by treating with 3-aminoazetidinone derivative III
with 4-[Me3CO2CNHCH(CO2Me)CH2CH2O]C6H4COCO2H and deblocking. III was obtained from 2-thienylglycine Me ester in 5 steps. I (X = O) had a min. inhibitory concentration, against Escherichia coli, of 0.5 μg/mL.
IT 63855-48-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)
RN 63855-48-1 CAPLUS

L4 ANSWER 192 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1-Azetidineacetic acid, 3-[[(hydroxyimino)phenylacetyl]amino]-2-oxo-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

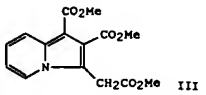


L4 ANSWER 193 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:72390 CAPLUS
DOCUMENT NUMBER: 86:72390
TITLE: Addition reactions of heterocyclic compounds. Part LXV. Synthesis, tautomerism, and rearrangement of some 2H- and 4H-quinolizine esters
AUTHOR(S): Acheson, R. Morrin; Hodgson, Stephen J.; Wright, R. Gordon McR.
CORPORATE SOURCE: Dep. Biochem., Univ. Oxford, Oxford, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (18), 1911-15
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

II

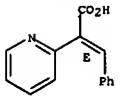


III

AB Alkaline hydrolysis and decarboxylation of tetra-Me 4H-quinolizine-1,2,3,4-
tetracarboxylates gave tri-Me 2H and 4H-quinolizine-1,2,3-tricarboxylates which were interconverted under PhMe reflux. E.g., I (R = CO2Me) with M NaOH in MeCN followed by decarboxylation with M HCl gave I (R = H) and II (R = CO2Me, R1 = Me). The nonequivalence of the 4-protons in the 4H-isomers at low temps. is associated with an sp2-hybridized N atom and restricted rotation of the ester groups. The quinolizines with HNO3 or PhOH gave indolizines. E.g., I (R = H) and II (R = CO2Me, R1 = Me) with PhOH gave 71 and 64% indolizine III, resp. Et 2-(2-pyridyl)cinnamate (IV)
with acetylenecarboxylates gave 2H-quinolizines. E.g., IV with HC.tplbond.CCO2Me gave II (R = Ph, R1 = Et).
IT 24864-32-2P 61860-38-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with di-Me acetylenedicarboxylate and Me propiolate)
RN 24864-32-2 CAPLUS
CN 2-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

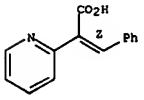
Double bond geometry as shown.

L4 ANSWER 193 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

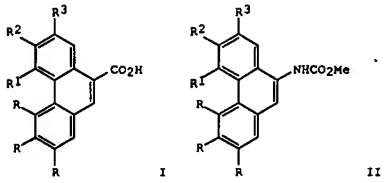


RN 61860-38-6 CAPLUS
CN 2-Pyridineacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

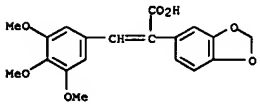
Double bond geometry as shown.



L4 ANSWER 194 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:577119 CAPLUS
DOCUMENT NUMBER: 85:177119
TITLE: Nonsymmetric 9-phenanthrylamines. An improved synthetic procedure to a useful synthon
AUTHOR(S): Krow, Grant; Damodaran, Kalyani M.; Michener, Edward; Miller, Stephen I.; Dalton, David R.
CORPORATE SOURCE: Dep. Chem., Temple Univ., Philadelphia, PA, USA
SOURCE: Synthetic Communications (1976), 6(4), 261-7
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:177119
GI



AB 9-Phenanthrenecarboxylic acids I [R = OMe, R1 = H, R2R3 = (CH2O2); R = R3 = H, R1R2 = (CH2O2); R = R1 = R2 = R3 = H] reacted with diphenylphosphoryl azide and Me3SiN3 in MeOH to yield the resp. Me N-(9-phenanthryl)carbamates (II).
IT 60848-05-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, phenanthrene derivative from)
RN 60848-05-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(3,4,5-trimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



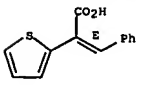
L4 ANSWER 194 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 195 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:514443 CAPLUS
DOCUMENT NUMBER: 83:114443
TITLE: Cephalosporin and penicillin antibiotics
INVENTOR(S): Gregory, Gordon I.; Gregson, Michael; Webb, Godfrey Basil
PATENT ASSIGNEE(S): Glaxo Laboratories Ltd., UK
SOURCE: Ger. Offen., 73 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2457358	A1	19750612	DE 1974-2457358	19741204
GB 1497039	A	19780105	GB 1973-56460	19731205
US 4014869	A	19770329	US 1974-528944	19741202
BE 822933	A1	19750604	BE 1974-151143	19741204
NL 7415792	A	19750609	NL 1974-15792	19741204
DK 7406305	A	19750721	DK 1974-6305	19741204
JP 50105688	A	19750820	JP 1974-138550	19741204
CA 1056373	A1	19790612	CA 1974-215228	19741204
CH 618440	A5	19800731	CH 1974-16109	19741204
FR 2253516	A1	19750704	FR 1974-39864	19741205
FR 2253516	B1	19790928		
AU 7476126	A	19760610	AU 1974-76126	19741205
PRIORITY APPLN. INFO.:			GB 1973-56460 A	19731205

GI For diagram(s), see printed CA Issue.
AB Cephalosporins I (R = Ph, AcOCH2, 2-furyl, MeOCH2, R1 = Ph; R = 2-thienyl, R1 = Ph, 2-thienyl; R = Ph, Me, Et, 4-NCC6H4, PhCH2CH2, R1 = 2-thienyl; R2 = OAc, 2-benzothiazolylthio, 5-methyl-1,3,4-thiadiazol-2-ylthio, O2CNH2, pyridinium) and the penicillins II (R = Me, R1 = Ph; R = Ph, R1 = 2-thienyl, 2-furyl) were prepared by acylating the 7-aminocephalosporanic acids or 6-aminopenicillanic acid with the cis-propanoic acids or their chlorides.
IT 38313-33-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of aminocephalosporanate by)
RN 38313-33-6 CAPLUS
CN 2-Thiopheneacetic acid, α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

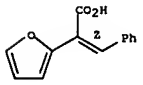
Double bond geometry as shown.



IT 57200-20-1P 57200-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

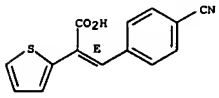
L4 ANSWER 195 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(prepn. and acylation of aminocephalosporanates by)
RN 57200-20-1 CAPLUS
CN 2-Furanacetic acid, α-(phenylmethylene)-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

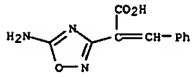


RN 57200-22-3 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-cyanophenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

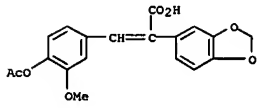
Double bond geometry as shown.



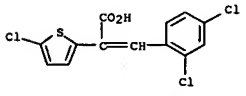
L4 ANSWER 196 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:156187 CAPLUS
DOCUMENT NUMBER: 82:156187
TITLE: Preparation of 3-substituted 5-amino-1,2,4-oxadiazoles from amidoximes with cyanogen bromide
AUTHOR(S): Dost, Johannes; Leisner, Rudi
CORPORATE SOURCE: Sekt. Chem./Biol., Paedagog. Hochsch. "Wolfgang Ratke", Koethen, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (1975), 15(2), 57
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 82:156187
GI For diagram(s), see printed CA Issue.
AB Oxadiazoles I (R = Me, Ph, PhCH2, PhCH:CH, Ph(CH:CH)2, Me2NC6H4CH:CH, HO2CCH2, PhCH:CHCH:C(CO2R1), MeOC6H4CH:C(CO2R1), Me2NC6H4CH:C(CO2R1), R1 = H, R) were prepared in 60-5% yield by treating RC(:NOH)NH2 with BrCN. RC(:NOH)NH2 were prepared from RCN and NH2OH.
IT 55654-08-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 55654-08-5 CAPLUS
CN 1,2,4-Oxadiazole-3-acetic acid, 5-amino-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



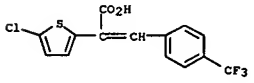
L4 ANSWER 197 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:31062 CAPLUS
DOCUMENT NUMBER: 82:31062
TITLE: Lignin chromophores. I. Synthesis of chromophores of the 2,4'- and 4,4'-dihydroxystilbene types
AUTHOR(S): Gierer, Josef; Lenic, Joze; Noren, Isa; Szabo-Lin, Ilona
CORPORATE SOURCE: Chem. Dep., Swedish Forest Prod. Res. Lab., Stockholm, Swed.
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1974), 28(7), 717-29
CODEN: ACBOCV; ISSN: 0302-4369
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Stilbenediols I and II and their hydroxymethyl derivs. III and IV were prepared by Knoevenagel condensation of 2,4,3-RR1(MeO)C6H2CHO acetate with 3,4-(MeO)(AcO)C6H3CH2CO2H (V) followed by decarboxylation and deacetylation to give I and II, or by esterification and reduction to give III and IV. Thus, Knoevenagel condensation of V with 4,3-(AcO)(MeO)C6H3CHO or 2,3-(AcO)(MeO)C6H3CHO in Ac2O and Et3N gave the acids VI and VII, resp. which were decarboxylated with Cu chromite and hydroquinone in quinoline, then deacetylated with LiAlH4 in THF to give I and II. Esterification of VI and VII with CH2N2 in dioxane, followed by reduction with LiAlH4 in THF gave III and IV.
IT 54208-15-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(decarboxylation of)
RN 54208-15-0 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[[4-(acetyloxy)-3-methoxyphenyl]methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 198 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:514392 CAPLUS
DOCUMENT NUMBER: 81:114392
TITLE: Naphthothiophenes. 4. Preparation of multisubstituted 4-naphtho[2,1-b]thiophenemethanols and the effect of side chain modification on antimalarial activity of 8-trifluoromethyl-4-naphtho[2,1-b] thiophenemethanols
AUTHOR(S): Das, Bijan P.; Nuss, Merrill E.; Boykin, David W., Jr.
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, GA, USA
SOURCE: Journal of Medicinal Chemistry (1974), 17(5), 516-19
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Of a series of 18 title compds. prepared and tested for antimalarial activity in mice, 2-chloro-8-(trifluoromethyl)-α-(N,N-dibutylaminomethyl)-4-naphtho[2,1-b]thiophenemethanol-HCl (I) [52300-69-3] gave cures against Plasmodium berghei at 80 mg/kg dose levels. I was prepared from α-(5-chloro-2-thienyl)-β-(p-trifluoromethylphenyl)acrylic acid [52300-53-5] by photocyclization followed by a conventional 5 step route involving the bromomethyl ketone intermediate. The effect of substituents on activity is discussed.
IT 52300-52-4P 52300-53-5P 52300-54-6P
52300-55-7P 52300-56-8P 52300-96-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52300-52-4 CAPLUS
CN 2-Thiopheneacetic acid, 5-chloro-α-[(2,4-dichlorophenyl)methylene]- (9CI) (CA INDEX NAME)

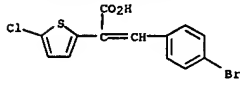


RN 52300-53-5 CAPLUS
CN 2-Thiopheneacetic acid, 5-chloro-α-[[4-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)

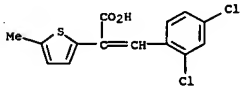


RN 52300-54-6 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-bromophenyl)methylene]-5-chloro- (9CI) (CA INDEX NAME)

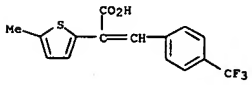
L4 ANSWER 198 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



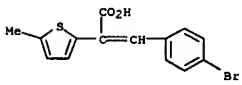
RN 52300-55-7 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2,4-dichlorophenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)



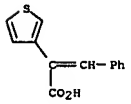
RN 52300-56-8 CAPLUS
CN 2-Thiopheneacetic acid, 5-methyl-α-[[4-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 52300-96-6 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-bromophenyl)methylene]-5-methyl- (9CI) (CA INDEX NAME)

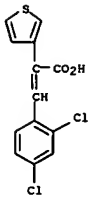


L4 ANSWER 199 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:10502 CAPLUS
DOCUMENT NUMBER: 80:10502
TITLE: Naphthothiophenes. 3. Preparation of 4-naphtho[1,2-b]thiophenemethanols and 5-naphtho[1,2-b]thiophenemethanols and attempts to prepare 5-naphtho[2,1-b]thiophenemethanols as antimalarials
AUTHOR(S): Das, Bijan P.; Cunningham, Robert T.; Boykin, David W., Jr.
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, GA, USA
SOURCE: Journal of Medicinal Chemistry (1973), 16(12), 1361-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Seven α-(N,N-dialkylaminomethyl)-4-and five α-(N,N-dialkylaminomethyl)-5-naphtho[1,2-b]thiophenemethanols were prepared and screened for antimalarial activity. In the 4-naphtho[1,2-b]thiophenemethanol series the di-n-heptylamino side chain exhibited greater activity than the dibutylamino side chain whereas in the 5-naphtho[1,2-b]thiophenemethanol series the converse was observed Six compds. gave cures against Plasmodium berghei in mice, α-(dibutylaminomethyl)-8-trifluoromethyl-5-naphtho[1,2-b]thiophenemethanol-HCl (I) [49561-91-3] being the most active compound I
gave cures against P. berghei at 160 mg/kg and was active at 10 mg/kg. I was active against P. gallinaceum at 320 mg/kg.
Naphtho[1,2-b]thiophene-4- and naphtho[1,2-b]thiophene-5-carboxylic acids, prepared by photooxidative
cyclization of δ-(3-thienyl)-β-acrylic acids and α-aryl-β-(3-thienyl)acrylic acids, resp., were converted into the title compds. by a 5-step route involving bromomethyl ketone intermediates.
IT 50920-07-5P 50920-08-6P 50920-09-7P
50920-10-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50920-07-5 CAPLUS
CN 3-Thiopheneacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)

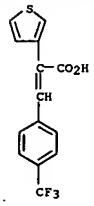


RN 50920-08-6 CAPLUS
CN 3-Thiopheneacetic acid, α-[[4-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)

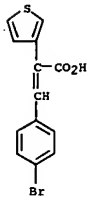
L4 ANSWER 199 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 199 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



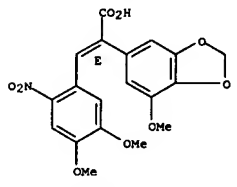
RN 50920-09-7 CAPLUS
CN 3-Thiopheneacetic acid, α-[(4-bromophenyl)methylene]- (9CI) (CA INDEX NAME)



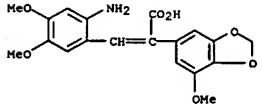
RN 50920-10-0 CAPLUS
CN 3-Thiopheneacetic acid, α-[(2,4-dichlorophenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 200 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:491828 CAPLUS
DOCUMENT NUMBER: 79:91828
TITLE: Synthesis of 2,6,7-trimethoxy-3,4-methylenedioxyphenanthrene, a degradation product of ocoteine
AUTHOR(S): Moltrasio, Graciela Y.; Giacopello, D.; Vernengo, M. J.
CORPORATE SOURCE: Dep. Quim. Org., Fac. Cienc. Exactas Nat., Buenos Aires, Argent.
SOURCE: Australian Journal of Chemistry (1973), 26(9), 2035-9
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2,6,7-Trimethoxy-3,4(methylenedioxy)phenanthrene (I) prepared by the Pschorr
reaction, is the same product obtained by degradation of ocoteine (II).
IT 42527-87-7P 42527-88-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42527-87-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(4,5-dimethoxy-2-nitrophenyl)methylene]-7-methoxy-, (E)- (9CI) (CA INDEX NAME)

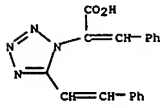
Double bond geometry as shown.



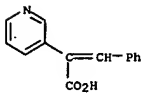
RN 42527-88-8 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[(2-amino-4,5-dimethoxyphenyl)methylene]-7-methoxy- (9CI) (CA INDEX NAME)



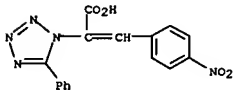
L4 ANSWER 201 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:136166 CAPLUS
DOCUMENT NUMBER: 78:136166
TITLE: Reactions of 4-arylidene-2-styryl-5(4)-oxazolones and related compounds
AUTHOR(S): Fahmy, A. F. M.; Orabi, M. O. A.
CORPORATE SOURCE: Chem. Dep., Ain Shams Univ., Cairo, Egypt
SOURCE: Indian Journal of Chemistry (1972), 10(10), 961-4
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 4-Arylidene-2-styryl-5(4)-oxazolones (I, R = H, Me) reacted with benzene in the presence of anhydrous AlCl3 to give PhCOCH2NHCOCH:CPh2. o-H2NC6H4CO2H with I (R = H, Me) gave p-RC6H4CH:C(NHCOCH:CHPh)CONHR1 (II, R = H, Me, R1 = o-HO2CC6H4) but p-aminobenzoic acid gave the imidazolones (III, R = H, Me; R1 = p-HO2CC6H4). I reacted with m-aminobenzoic acid to give III(R = H, R1 = m-HO2CC6H4) and II (R = Me, R1 = m-HO2CC6H4). I also underwent aminolysis, alcoholysis hydrolysis, hydrazinolysis and azidolysis to give cleavage products which were characterized on the basis of elemental analysis and ir data.
IT 40913-24-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40913-24-4 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-(2-phenylethenyl)-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



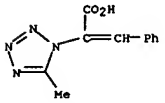
L4 ANSWER 202 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:67618 CAPLUS
DOCUMENT NUMBER: 78:67618
TITLE: Potential hypolipidemic agents. III. Heterocyclic compounds affecting free fatty acid mobilization in vivo
AUTHOR(S): Carlson, Lars A.; Hedbom, Christina; Helgstrand, Erik; Sjoberg, Berndt; Stjernstrom, Nils E.
CORPORATE SOURCE: King Gustaf Vth Res. Inst., Stockholm, Swed.
SOURCE: Acta Pharmaceutica Suecica (1972), 9(4), 289-304
CODEN: APSXAS; ISSN: 0001-6675
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Compds. such as 3-methyl-5-isoxazolecarboxylic acid [4857-42-5], 5-fluoronicotinic acid [402-66-4], 5-fluoro-3-pyridylacetic acid [38129-24-7], and 3-methylpyrazole [1453-58-3] exhibited the highest inhibition of free fatty acid mobilization in blood among 188 heterocyclic compds. tested in dogs, while compds. such as 5-methyl-3-isoxazolecarboxylic acid [3405-77-4], 2-fluoronicotinic acid [393-55-5], and 3-aminobenzoic acid [99-05-8] had no effect on free fatty acid mobilization.
IT 32967-19-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(lipid metabolism inhibition by)
RN 32967-19-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



L4 ANSWER 203 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:58328 CAPLUS
DOCUMENT NUMBER: 78:58328
TITLE: Thermolysis of derivatives of β-substituted α-(1-tetrazolyl)acrylic acids. I. Formation of some imidazolones and a thiazolone
AUTHOR(S): Lykkeberg, Jytte; Klitgaard, Niels Anders
CORPORATE SOURCE: Chem. Lab. C., R. Dan. Sch. Pharm., Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1972), 26(7), 2687-94
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new method of preparing unsatd. 5-imidazolones (2-substituted 4-arylmethylene-4-imidazolones) involving Cu-catalyzed thermolysis of β-substituted α-(1-tetrazolyl)acrylamides was developed. Transformation of a β-substituted α-(1-tetrazolyl)thioloacrylic acid to the unsatd. 5-thiazolone was accomplished by heating alone but the product was contaminated with the corresponding oxazolone. Attempts to prepare an as-triazine by heating of a β-substituted α-(1-tetrazolyl)acrylohydrazide only led to the corresponding 1-vinyltetrazole.
IT 1738-45-0 1738-50-7 1738-65-4
36194-90-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)
RN 1738-45-0 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[(4-nitrophenyl)methylene]-5-phenyl- (9CI) (CA INDEX NAME)

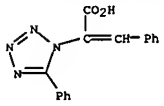


RN 1738-50-7 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

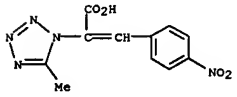


RN 1738-65-4 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-phenyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

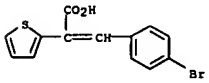
L4 ANSWER 203 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



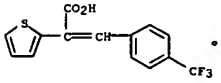
RN 36194-90-8 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-methyl-α-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)



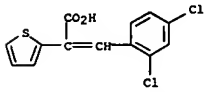
L4 ANSWER 204 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:413966 CAPLUS
DOCUMENT NUMBER: 77:13966
TITLE: Naphthothiophenes. 1. α-(Alkylaminomethyl)-4-naphtho[2,1-b]thiophenemethanols as antimalarials
AUTHOR(S): Das, B. P.; Campbell, J. A.; Samples, F. B.; Wallace, R. A.; Whisenant, L. K.; Woodard, R. W.; Boykin, D. W., Jr.
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, GA, USA
SOURCE: Journal of Medicinal Chemistry (1972), 15(4), 370-4
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 77:13966
AB A series of substituted alkylaminomethylnaphtho[2,1-b]thiophene-4-methanols (I) were synthesized by photooxidative cyclization of arylthienylethylenes followed by attachment of α-[(dibutylamino)methyl]- and α-(N-piperidinomethyl)- side chains via a classical 5-step procedure involving diazo ketone intermediates. α-[(Dibutylamino)methyl]-8-trifluoromethylnaphtho[2,1-b]thiophene-4-methanol-HCl [34861-50-2] (I, R = CF3, R1 = H, R2 = CH2NBu2 HCl salt) and α[(dibutylamino)methyl]-6,8-dichloronaphtho[2,1-b]thiophene-4-methanol-HCl [34861-51-3] (I, R = R1 = Cl, R2 = CH2NBu2 HCl salt) showed antimalarial activity against Plasmodium berghei in mice. No activity was observed for compds. bearing the α-(N-piperidinomethyl) side chain.
IT 37094-46-5P 37094-47-6P 37094-48-7P
38313-33-6P 38343-87-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 37094-46-5 CAPLUS
CN 2-Thiopheneacetic acid, α-[(4-bromophenyl)methylene]- (9CI) (CA INDEX NAME)



RN 37094-47-6 CAPLUS
CN 2-Thiopheneacetic acid, α-[[4-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)

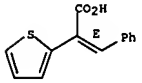


L4 ANSWER 204 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 37094-48-7 CAPLUS
CN 2-Thiopheneacetic acid, α-[(2,4-dichlorophenyl)methylene]- (9CI) (CA INDEX NAME)



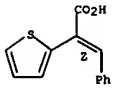
RN 38313-33-6 CAPLUS
CN 2-Thiopheneacetic acid, α-(phenylmethylene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

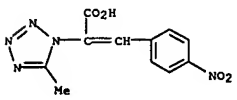


RN 38343-87-2 CAPLUS
CN 2-Thiopheneacetic acid, α-(phenylmethylene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 205 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:140666 CAPLUS
DOCUMENT NUMBER: 76:140666
TITLE: Synthesis of some new ω-substituted 1-vinyltetrazole derivatives
AUTHOR(S): Lykkeberg, Jytte; Klitgaard, Niels A.
CORPORATE SOURCE: Chem. Lab., R. Dan. Sch. Pharm., Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1972), 26(1), 266-74
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 76:140666
AB Azidolytic transformation of 5-oxazolones followed by a Cu-quinoline induced decarboxylation of the resulting α-(1-tetrazolyl)acrylic acids gave 1,5-disubstituted tetrazoles. In some cases the decarboxylation procedure gave a mixture of the cis and trans isomers of the tetrazoles.
IT 36194-90-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36194-90-8 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-methyl-α-[(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)

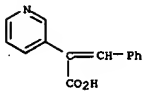


L4 ANSWER 206 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:463630 CAPLUS
DOCUMENT NUMBER: 75:63630
TITLE: Antiinflammatory 3-substituted 2-pyridone and 2-thiopyridone derivatives
INVENTOR(S): Shen, Tsung-Ying; Walford, Gordon L.; Witzel, Bruce E.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Ger. Offen., 61 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

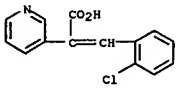
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2059358	A	19710609	DE 1970-2059358	19701202
NL 7016899	A	19710607	NL 1970-16899	19701118
JP 49039267	B	19741024	JP 1970-103716	19701126
CH 577475	A5	19760715	CH 1970-17636	19701126
CA 945991	A1	19740423	CA 1970-99369	19701127
GB 1289187	A	19720913	GB 1970-1289187	19701201
FR 2081325	A5	19711203	FR 1970-43348	19701202
FR 2081325	B1	19750110		
US 3846553	A	19741105	US 1971-172319	19710816
PRIORITY APPLN. INFO.:			US 1969-881922 A	19691203

GI For diagram(s), see printed CA Issue.
AB Title compds. were prepared by oxidation of the appropriately substituted pyridine with peroxide, and heating the pyridine N-oxide formed with an acid anhydride. Treatment of a 2-pyridone compound with a strong base and addition of an appropriate aliphatic or aromatic compound gives N-substituted products, converted by heating with P2S5 into the corresponding N-substituted thiopyridones. Thus, equimolar amts. 3-HOC5H4N and KOH heated at 150° (in a stream of N and the product treated with 3-HOC5H4N and CuCO3 in PhBr, and the mixture heated 3 hr at 150° and 15 hr at 180° gave 3-PhOC5H4N. This in AcOH heated 15 hr at 75° with 30% H2O2 gave 3-PhOC5H4NO, which refluxed 5 hr in Ac2O gave 3-phenoxy-2[(1H]-pyridone. trans-3-(o-Chlorostyryl)-2[1H]-pyridone treated with NaH in DMF 2.5 hr at 45° and the ice-cold mixture treated with BrCH2C.tplbond.CH, then stirred 10 hr at 20° gave I. trans-3-(o-Chlorostyryl)-2[1H]-pyridone in dry C5H5N refluxed with P2S5 gave trans-3-(o-chlorostyryl)-2[1H]-thipyridone.
IT 32967-19-4P 32967-20-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 32967-19-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)

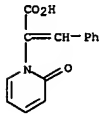
L4 ANSWER 206 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



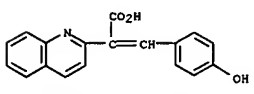
RN 32967-20-7 CAPLUS
CN 3-Pyridineacetic acid, α-(o-chlorobenzylidene)- (8CI) (CA INDEX NAME)



L4 ANSWER 207 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:435259 CAPLUS
DOCUMENT NUMBER: 73:35259
TITLE: Anhydro-2-hydroxyoxazolo[3,2-a]pyridinium hydroxide, a mesoionic oxazolone
AUTHOR(S): Boyd, Gerhard V.; Wright, Peter Hannan
CORPORATE SOURCE: Dep. Chem., Chelsea Coll. Sci. Technol., London, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (10), 1485-90
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Treatment of 1,2-dihydro-2-oxopyridine-1-acetic acid with Ac2O and perchloric acid yields 2,3-dihydro-2-oxooxazolo[3,2-a]pyridinium perchlorate, which is deprotonated by Et3N in CH2Cl2 to give the highly labile anhydro-2-hydroxyoxazolo[3,2-a]pyridinium hydroxide in solution Stable acyl and azo derivs. of this mesoionic compound are obtained by electrophilic substitution reactions; amines open the oxazolone ring with the formation of amides of 1,2-dihydro-2-oxopyridineacetic acid. The oxazolopyridinium perchlorate condenses with aromatic aldehydes to give colored arylidene derivs.; the salicylidene compound readily rearranges to a coumarin. Coumarins are also obtained by reaction of the mesoionic base with o-hydroxyarene-carboxaldehydes. The dimeric decomposition product of the mesoionic oxazolone is the 3-[(1,2-dihydro-2-oxo-1-pyridyl)acetyl] derivative
IT 27329-06-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27329-06-2 CAPLUS
CN 1(2H)-Pyridineacetic acid, α-benzylidene-2-oxo- (8CI) (CA INDEX NAME)

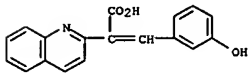


L4 ANSWER 208 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:43386 CAPLUS
DOCUMENT NUMBER: 72:43386
TITLE: Heterocyclic compounds. II. Condensation of 2-quinolylacetic acid hydrochloride, and 2-, and 4-quinolylpyruvates with aromatic aldehydes
AUTHOR(S): Al-Tai, F. A.; Sarkis, George Y.; Al-Najjar, F. A.
CORPORATE SOURCE: Coll. Sci., Baghdad, Iraq
SOURCE: Bulletin of the College of Science, University of Baghdad (1967), 10, 93-101
CODEN: BCOSAF; ISSN: 0408-1927
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2-Quinolylacetic acid-HCl was condensed with substituted benzaldehydes in aqueous alc. at 55-70° to give the following I (R, m.p., % yield, and m.p . picrate given): Ph, 271-2°, 66, 133°; p-O2NC6H4, 290-1°, 68, -; p-HOC6H4, 269-70°, 26, -; m-HOC6H4, 289-90°, 33, -. 2-Quinolylpyruvic acid-HCl is similarly condensed with aldehydes to give the following II (R, m.p., % yield, and m.p. 2,4-di-nitrophenylhydrazone given): Ph, 245-6°, 74, 124-5°; p-O2N-C6H4, 265-6°, 71, 145-6°; m-O2NC6H4, 256-7°, 51, 140-1°; quinolyl, 236-7°, 50, 156-7°. 4-Quinolylpyruvic acid-HCl and p- and m-O2NC6H4CHO similarly gave 56% 2-γ-quinolyl-3-p-(m. 249-50°; 2,4-dinitrophenylhydrazone m. 164-5°) and 50% 3-m-nitrophenyl-3-hydroxypropanal (m. 260-1°, 2,4-dinitrophenylh ydrazone m. 152-3°), resp. On heating with p- or m-O2NC6H4CHO and piperidine for 24 hr, Et 2-quinolylpyruvate (III) gives, resp., 75% Et 4-(p- and 50% Et 4-(m-nitrophenyl)-3-α-quinolyl-2-oxo-3-butenoate (m. 198-9°, red, and 218-19°, yellow, resp.). Similarly, Et 4-quinolylpyruvate (IV) and p-O2NC6H4CHO in piperidine gives 50% ethyl 4-(p-nitrophenyl)-3-γ-quinolyl-2-oxo-3-butenoate (dark red, m. 210-12°). Ph-CHO, m-HOC6H4CHO, and p-HOC6H4CHO do not react with IV when they are heated together at 70-80° for 15 hr. III (53%; m. 131-2°, picrate m. 156-7° (decomposition) and 48% IV (m. 196-7°; picrate m. 207-8°; 2,4-dinitrophenylhydrazone m. 177°) were prepared by the condensation of quinaldine and (EtO2C)2 in alc. ether in the presence of NaOEt. In the condensation of 2- and 4-quinolylpyruvic acid hydrochlorides with BzH and its derivs., the temperature required is lower than in the condensation of pyridyl- and quinolylacetic acid hydrochlorides. This is attributed to the reactive methylene groups in α-keto acids.
IT 25888-36-2P 25888-37-3P 25888-69-1P 25888-70-4P 25888-71-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 25888-36-2 CAPLUS
CN 2-Quinolineacetic acid, α-(p-hydroxybenzylidene)- (8CI) (CA INDEX NAME)

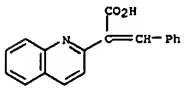


RN 25888-37-3 CAPLUS

L4 ANSWER 208 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Quinolineacetic acid, α-(m-hydroxybenzylidene)- (8CI) (CA INDEX NAME)



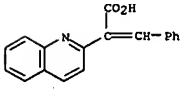
RN 25888-69-1 CAPLUS
CN 2-Quinolineacetic acid, α-benzylidene- (8CI) (CA INDEX NAME)



RN 25888-70-4 CAPLUS
CN 2-Quinolineacetic acid, α-benzylidene-, picrate (8CI) (CA INDEX NAME)

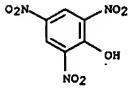
CM 1

CRN 25888-69-1
CMF C18 H13 N O2



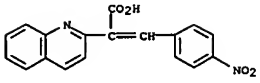
CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



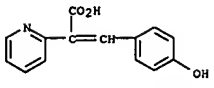
RN 25888-71-5 CAPLUS
CN 2-Quinolineacetic acid, α-(p-nitrobenzylidene)- (8CI) (CA INDEX NAME)

L4 ANSWER 208 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

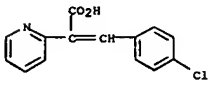


L4 ANSWER 209 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:43377 CAPLUS
DOCUMENT NUMBER: 72:43377
TITLE: Heterocyclic compounds. I. Condensation of 2-, and 4-pyridylacetic acid hydrochlorides with carbonyl compounds
AUTHOR(S): Al-Tai, F. A.; Sarkis, George Y.; Al-Najjar, F. A.
CORPORATE SOURCE: Coll. Sci., Baghdad, Iraq
SOURCE: Bulletin of the College of Science, University of Baghdad (1967), 10, 81-92
CODEN: BCOSAF; ISSN: 0408-1927
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Et 2-pyridylacetate condenses with BzH in alc. in the presence of piperidine on 10 hr refluxing to afford 43% Et trans-α-2-pyridylcinnamate (I) (b4.5 194-5°); free acid m. 156-7°. When 2- and 4-pyridylacetic acid hydrochlorides were treated with substituted benzaldehydes in aqueous alc. at pH 6 and at 45-50° (4-6 hr), dehydration occurred, to give II and III, resp. The following II and III were prepared (Ar, m.p. I, % yield I, m.p. I picrate, m.p. II, % yield II and m.p. II picrate given): Ph, 10 7-8°, 75, -, 136-7°, 38, -; o-O2NC6H4, 138-9°, 83, 144-5°, 144-5°, 44, 198-200°; m-O2NC6H4, 82-3°, 66, -, 125-7°, 39, -; p-O2NC6H4, 164-5°, 91, 178-9°, 171-2°, 75, -; m-HOC6H4, 90-1°, 38, 217-8°, 113-14°, 28, 227-8°. II and III and their picrates are yellow to brown, all from alc. II (Ar = Ph) and in refluxing C6H6 with PCl5 gave 62% β-2-pyridylstyrene, m. 89-90° (picrate m. 207°); similarly prepared was 41% β-4-pyridylstyrene, m. 127°; picrate m. 113°. Condensation of 2-pyridylacetic and 4-pyridylacetic acids with p-ClC6H4CHO and p-HOC6H4CHO at pH 6 gives α-pyridylcinnamic acids (IV and V, resp.) as follows (R, m.p. IV, % yield, m.p. IV picrate, m.p. V, % yield, and m.p. V picrate given): Cl, 130-1°, 51, 147-8°, 13 9-40°, 43, 106°; HO, 110-11°, 47, 230-1°, 195-6°, 30, 244-5. Decreased electron d. at the o-and p-positions increases the rate and yield of condensation. Electron donors stabilize the acid intermediate. A mechanism of the condensation is presented.
IT 20093-37-2P 20093-38-3P 24832-34-6P 24832-37-9P 24832-46-0P 24843-18-3P 24843-19-4P 24843-22-9P 24864-32-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20093-37-2 CAPLUS
CN 2-Pyridineacetic acid, α-(p-hydroxybenzylidene)- (8CI) (CA INDEX NAME)

L4 ANSWER 209 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



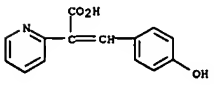
RN 20093-38-3 CAPLUS
CN 2-Pyridineacetic acid, α-(p-chlorobenzylidene)- (8CI) (CA INDEX NAME)



RN 24832-34-6 CAPLUS
CN 2-Pyridineacetic acid, α-(p-hydroxybenzylidene)-, monopicrate (8CI) (CA INDEX NAME)

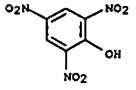
CM 1

CRN 20093-37-2
CMF C14 H11 N O3



CM 2

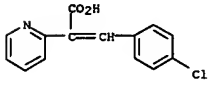
CRN 88-89-1
CMF C6 H3 N3 O7



RN 24832-37-9 CAPLUS
CN 2-Pyridineacetic acid, α-(p-chlorobenzylidene)-, monopicrate (8CI) (CA INDEX NAME)

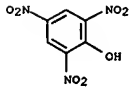
CM 1

L4 ANSWER 209 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 20093-38-3
CMF C14 H10 Cl N O2

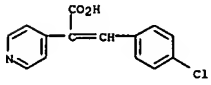


CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



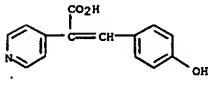
RN 24832-46-0 CAPLUS
CN 4-Pyridineacetic acid, α-(p-chlorobenzylidene)- (8CI) (CA INDEX NAME)



RN 24843-18-3 CAPLUS
CN 4-Pyridineacetic acid, α-(p-hydroxybenzylidene)-, monopicrate (8CI) (CA INDEX NAME)

CM 1

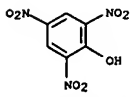
CRN 24843-19-4
CMF C14 H11 N O3



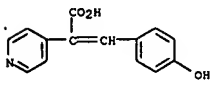
CM 2

L4 ANSWER 209 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 88-89-1
CMF C6 H3 N3 O7



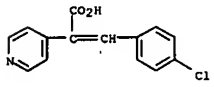
RN 24843-19-4 CAPLUS
CN 4-Pyridineacetic acid, α-(p-hydroxybenzylidene)- (8CI) (CA INDEX NAME)



RN 24843-22-9 CAPLUS
CN 4-Pyridineacetic acid, α-(p-chlorobenzylidene)-, monopicrate (8CI) (CA INDEX NAME)

CM 1

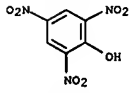
CRN 24832-46-0
CMF C14 H10 Cl N O2



CM 2

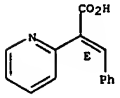
CRN 88-89-1
CMF C6 H3 N3 O7

L4 ANSWER 209 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 24864-32-2 CAPLUS
CN 2-Pyridineacetic acid, α-(phenylmethylene)-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 210 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

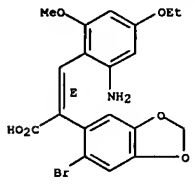
ACCESSION NUMBER: 1969:57515 CAPLUS
DOCUMENT NUMBER: 70:57515
TITLE: Plant constituents with a nitro group. VIII. Constitution of aristolochic acid IVa from Aristolochia argentina and Aristolochia clematitis
AUTHOR(S): Ruveda, Edmundo A.; Albonico, Sem M.; Priestap, H. A.; Deulofeu, Venancio; Pailer, Matthias; Goessinger, E.; Bergthaller, P.
CORPORATE SOURCE: Univ. Buenos Aires, Buenos Aires, Argent.
SOURCE: Monatsh. Chem. (1968), 99(6), 2349-58
CODEN: MOCHAP
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Aristolochic acid was identified as 3,4-methylenedioxy-6-hydroxy-8-methoxy - 10 - nitrophenanthrene - 1 - carboxylic acid by chemical degradation.

IT 21879-89-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 21879-89-0 CAPLUS
CN Acrylic acid, 3-(2-amino-4-ethoxy-6-methoxyphenyl)-2-[2-bromo-4,5-(methylenedioxy)phenyl]-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 211 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

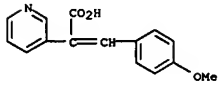
ACCESSION NUMBER: 1969:11514 CAPLUS
DOCUMENT NUMBER: 70:11514
TITLE: Heterocyclic analogs of pinosylvin
AUTHOR(S): Erdtman, Holger; Rosengren, Ake
CORPORATE SOURCE: Roy. Inst. Technol., Stockholm, Swed.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1968), 22(5), 1475-81
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

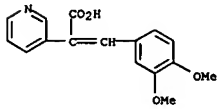
AB 3-Substituted stilbazole derivs. (I) were prepared by condensation of 3-pyridylacetic acid with methoxylated benzaldehydes followed by decarboxylation and demethylation. The synthetic procedures were studied in some detail. None of the hydroxylated stilbazoles showed any significant fungicidal activity as compared with pinosylvin (II).

IT 5847-83-6P 21000-55-5P 21000-57-7P 21000-58-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 5847-83-6 CAPLUS
CN 3-Pyridineacetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

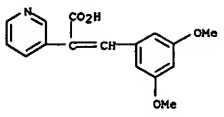


RN 21000-55-5 CAPLUS
CN 3-Pyridineacetic acid, α-[(3,4-dimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

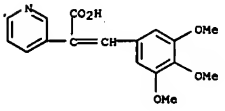


RN 21000-57-7 CAPLUS
CN 3-Pyridineacetic acid, α-[(3,5-dimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 211 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

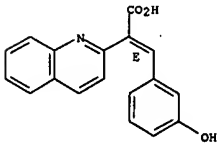


RN 21000-58-8 CAPLUS
CN 3-Pyridineacetic acid, α-(3,4,5-trimethoxybenzylidene)- (8CI) (CA INDEX NAME)



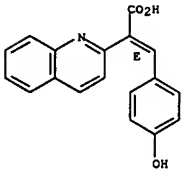
L4 ANSWER 212 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:506494 CAPLUS
DOCUMENT NUMBER: 69:106494
TITLE: Synthesis, ultraviolet, and infrared studies of heterocyclic compounds
AUTHOR(S): Al-Tai, F. A.; Sarkis, G. Y.; Al-Najjar, F. A.
SOURCE: Arab Sci. Congr., 5th, Bagdad (1966), Issue Pt. 2, 195-7. Editor(s): El-Tahrir, Midan. Amer. Univ. at Cairo: Cairo, UAR.
CODEN: 20ARAH
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Condensation of 2-, and 4-pyridylacetic acid hydrochlorides (I) and (II), at pH 6 with RC6H4CHO (III) (R = H, o-NO2, m-NO2, p-NO2, and m-OH) gave the corresponding 1-phenyl-1-hydroxy-2-(2-pyridyl)ethane and 1-phenyl-1-hydroxy-2-(4-pyridyl)ethane derivs. Other aldehydes such as III (R = p-Cl, p-OH) gave the corresponding cinnamic acid derivs. Condensation of I and II with isatin gave 3α-picolyldioxindole and 3-λ-picolyldioxindole. Condensation of 2-quinolylacetic acid hydrochloride at pH 6 with the same series of aldehydes afforded the corresponding cinnamic acid derivs. Et 2-, and 4-quinolylpyruvates were allowed to condense with a series of aromatic aldehydes using piperidine as a catalyst to obtain cinnamic acid derivs. Attempts to condense 2-, and 4-quinolylpyruvic acid hydrochlorides with aromatic aldehydes produced
derivs. of 1-quinolyl-2-hydroxy-2'-phenylpropionaldehyde. The ir and uv spectra of the above compds. were recorded.
IT 20374-16-7P 20374-17-8P 20374-18-9P
20374-19-0P 20374-20-3P 20374-21-4P
20374-22-5P 20374-24-7P 20374-25-8P
20374-26-9P 20374-28-1P 20698-39-9P
20698-40-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20374-16-7 CAPLUS
CN 2-Quinolineacetic acid, α-(m-hydroxybenzylidene)-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



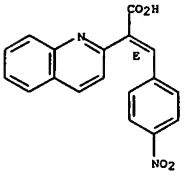
RN 20374-17-8 CAPLUS
CN 2-Quinolineacetic acid, α-(p-hydroxybenzylidene)-, (E)- (8CI) (CA INDEX NAME)

L4 ANSWER 212 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



RN 20374-18-9 CAPLUS
CN 2-Quinolineacetic acid, α-(p-nitrobenzylidene)-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

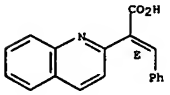


RN 20374-19-0 CAPLUS
CN 2-Quinolineacetic acid, α-benzylidene-, picrate, (E)- (8CI) (CA INDEX NAME)

CM 1

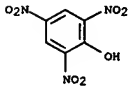
CRN 20374-20-3
CMF C18 H13 N O2

Double bond geometry as shown.



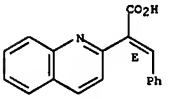
CM 2

L4 ANSWER 212 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 88-89-1
CMF C6 H3 N3 O7



RN 20374-20-3 CAPLUS
CN 2-Quinolineacetic acid, α-benzylidene-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

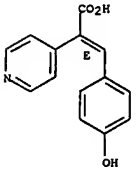


RN 20374-21-4 CAPLUS
CN 4-Pyridineacetic acid, α-(p-hydroxybenzylidene)-, picrate, (E)- (8CI) (CA INDEX NAME)

CM 1

CRN 20374-22-5
CMF C14 H11 N O3

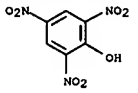
Double bond geometry as shown.



CM 2

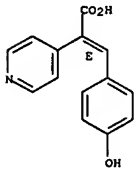
CRN 88-89-1
CMF C6 H3 N3 O7

L4 ANSWER 212 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



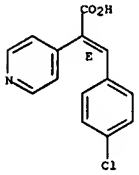
RN 20374-22-5 CAPLUS
CN 4-Pyridineacetic acid, α-(p-hydroxybenzylidene)-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 20374-24-7 CAPLUS
CN 4-Pyridineacetic acid, α-(p-chlorobenzylidene)-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

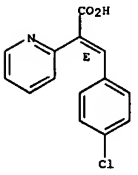


RN 20374-25-8 CAPLUS
CN 2-Pyridineacetic acid, α-(p-hydroxybenzylidene)-, picrate, (E)- (8CI) (CA INDEX NAME)

CM 1

L4 ANSWER 212 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Pyridineacetic acid, α-(p-chlorobenzylidene)-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

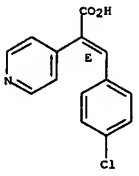


RN 20698-39-9 CAPLUS
CN 4-Pyridineacetic acid, α-(p-chlorobenzylidene)-, picrate, (E)- (8CI) (CA INDEX NAME)

CM 1

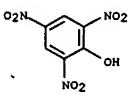
CRN 20374-24-7
CMF C14 H10 Cl N O2

Double bond geometry as shown.



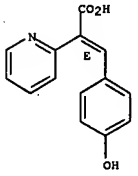
CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



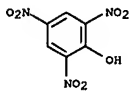
L4 ANSWER 212 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 20374-26-9
CMF C14 H11 N O3

Double bond geometry as shown.



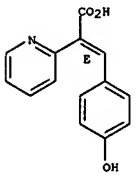
CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



RN 20374-26-9 CAPLUS
CN 2-Pyridineacetic acid, α-(p-hydroxybenzylidene)-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



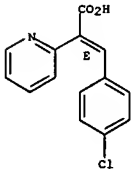
RN 20374-28-1 CAPLUS

L4 ANSWER 212 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 20698-40-2 CAPLUS
CN 2-Pyridineacetic acid, α-(p-chlorobenzylidene)-, picrate, (E)- (8CI) (CA INDEX NAME)

CM 1

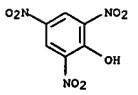
CRN 20374-28-1
CMF C14 H10 Cl N O2

Double bond geometry as shown.



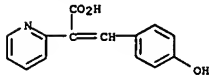
CM 2

CRN 88-89-1
CMF C6 H3 N3 O7

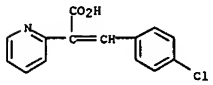


L4 ANSWER 213 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:506462 CAPLUS
DOCUMENT NUMBER: 69:106462
TITLE: Agents acting on the central nervous system. XI. Synthesis of methyl 3-phenyl-2-(2- and 4-pyridyl and piperidyl)-propionate and propanols
AUTHOR(S): Chatterji, S. K.; Mukerji, S.; Gautam, B. C.; Anand, Nitya
CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, India
SOURCE: Indian Journal of Chemistry (1968), 6(5), 235-8
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compds. were synthesized for evaluation of their pharmacol. activity. Thus, a mixture of 3.04 g. Me 4-pyridylacetate, 20 ml. Ac2O, and 8 ml. BzH was heated 6 hrs. on a water bath to yield 55% Me α-(4-pyridyl)cinnamate, m. 95°. A mixture of 2.44 g. BzH, 3.02 g. Me 2-pyridylacetate, 0.07 g. piperidine, and 0.25 g. HOAc was refluxed 12 hrs. (Dean-Stark separator) to yield Me α-(2-pyridyl)cinnamate (Ia). Ia (5 g.) in 50 ml. 4N HCl was heated 4 hrs. on a water bath and the mixture evaporated to dryness in vacuo. The residue was dissolved in a small quantity of H2O and applied to an IR-4B(OH) column (10 ml.). Elution with H2O and evaporation of the eluate yielded α-(2-pyridyl)cinnamic acid. Alternatively, 5 g. Ia was refluxed 3 hrs. with 25 ml. alc. NaOH, EtOH removed in vacuo, and the product worked up as above. The tabulated I were similarly prepared A solution of 12 g. Ia in 50 ml. MeOH was added to a pre-reduced suspension of 3.5 g. 10% Pd-C in 50 ml. MeOH and hydrogenation carried out at room temperature and atmospheric pressure until 1 mole H was absorbed to yield Me 2-(2-pyridyl)-3-phenylpropionate (II). II (7g.) was hydrogenated in 100 ml. HOAc in the presence of 10% Pd-C to yield Me 2-(2-piperidyl)-3-phenylpropionate. LiAlH4 reduction of Me 3-(p-hydroxyphenyl)-2-(2-pyridyl)propionate in ether or tetrahydrofuran yielded 3-(p-hydroxyphenyl)-2-(2-pyridyl)-1-propanol. The tabulated 3-phenyl-2-(2- and 4-pyridyl and piperidyl)-propionates (IIa) were prepared The following tabulated 3-phenyl-2-(2- and 4-pyridyl and piperidyl)propanols (III) were also prepared The compds. prepared were evaluated for their effects on gross behavior, motor activity, and the cardiovascular system. None of the compound showed any significant activity.
IT 20093-37-2P 20093-38-3P 20093-39-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20093-37-2 CAPLUS
CN 2-Pyridineacetic acid, α-(p-hydroxybenzylidene)- (8CI) (CA INDEX NAME)

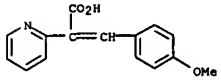
L4 ANSWER 213 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



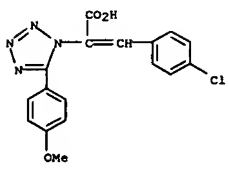
RN 20093-38-3 CAPLUS
CN 2-Pyridineacetic acid, α-(p-chlorobenzylidene)- (8CI) (CA INDEX NAME)



RN 20093-39-4 CAPLUS
CN 2-Pyridineacetic acid, α-(p-methoxybenzylidene)- (8CI) (CA INDEX NAME)



L4 ANSWER 214 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:443828 CAPLUS
DOCUMENT NUMBER: 69:43828
TITLE: The azidolysis of 4-arylidene and 4-alkylidene 5(4)-oxazolones. II
AUTHOR(S): Awad, William Ibrahim; Fahmy, Ameen Farouk Mohamed
CORPORATE SOURCE: Ain Shams Univ., Cairo, Egypt
SOURCE: Canadian Journal of Chemistry (1968), 46(13), 2207-16
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 69:43828
AB 4-Isopropylidene-5(4H)-oxazolones react with sodium azide in acetic acid in 5 min. or with hydrazoic acid in benzene to give the diazide Me2C(N3)CH(CON3)NHBz. The latter gives by thermolysis 3,4-dihydro-6-phenyl-4-isopropylidene-2-oxo-1,3,5-oxadiazine, which forms on hydrolysis the imide Me2CHCONHBz. The corresponding monoazides Me2C(CON3)NHBz react with sodium azide-acetic acid mixture to give the corresponding diazides. 4-Arylidene-5(4H)-oxazolones react under the same conditions to give α-(tetrazol-1-yl)acrylic acid derivs. The work of Deorha and Gupta (1965) is reinvestigated. The constitution of the products is discussed chemical and spectroscopically. 19 references.
IT 19747-12-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19747-12-7 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-chlorobenzylidene)-5-(p-methoxyphenyl)- (8CI) (CA INDEX NAME)



L4 ANSWER 215 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:482138 CAPLUS
DOCUMENT NUMBER: 67:82138
TITLE: Plant substances with a nitro group.. VI. Constitution of aristolochic acid-IV
AUTHOR(S): Pailer, Matthias; Bergthaller, P.
CORPORATE SOURCE: Univ. Vienna, Vienna, Austria
SOURCE: Monatshefte fuer Chemie (1967), 98(3), 579-91
CODEN: MOCHAP
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB cf. CA 65: 8842a. The structure of the title compound (I) was determined to be 6-nitro-8,10-dimethoxyphenanthro[3,4-d]-1,3-dioxole-5-carboxylic acid. The decarboxylation product of I (II) (loc. cit.) (18 g.) in 10 ml. tetrahydrofuran (THF) was boiled with 5 ml. 10% NH3 and 2 g. Zn. The mixture was filtered and the filtrate evaporated in vacuo. The residue was treated with 4 ml. THF and 2 ml. 5% HCl, followed by diazotization with 9 mg. NaNO2 at -2°. The mixture was treated with 3 ml. 60% H3PO2 and 10 mg. CuSO4 in 1 ml. water and kept 20 hrs. at 0° to give 1,3-dimethoxy-5,6-methylenedioxyphenanthrene (III), m. 138-42°; picrate m. 176-7°. II reduced over Pd-charcoal, followed by acetylation with Ac2O, gave 1,3-dimethoxy-5,6-methylenedioxy-9-acetamidophenanthrene (IV), decomposing 293-5°. Several degradation products of I were synthesized. 4,3,5-Me(O2N)2C6H2OH (13.7 g.) in 50 ml. HCONMe2 was treated with 65 g. K2CO3 and 29.5 ml. Me2SO4 to give 80% 4,3,5-Me(O2N)2C6H2OMe (V), m. 102-3°. V (23.8 g.) in 200 ml. AcOH was treated dropwise with 76.7 g. SnCl2 in 150 ml. HCl-saturated EtOH to give 4.3 g. 4,5,3-Me(H2N)(O2N)C6H2OMe (VI), m. 84-6°. VI was diazotized as usual. The diazotization product was treated with urea, followed by the addition of dilute H2SO4 at 100° and of 2 g. CuSO4 to give 88% 2,3,5-Me(HO)(MeO)C6H2NO2, which was converted into 2,3,5-Me(MeO)2C6H2NO2 (VII), m. 92-3°. A stirred and irradiated mixture of 4 g. VII, 3.9 g. N-bromosuccinimide, and 50 ml. CCl4 was kept until the temperature reached 55° to give 2,3,5-(BrH2C)(MeO)2C6H2NO2, m. 83°, which upon refluxing with 20 ml. dry C6H6 and 10 ml. absolute pyridine 2 hrs. gave 82% 1-(2-nitro-4,6-dimethoxybenzyl)pyridinium bromide (VIII); picrate m. 153-4°. A mixture of 5.9 g. VIII, 80 ml. iso-PrOH, and 3.3 g. 4-ONC6H4NMe2 was treated with 2 portions of 2 g. NaOH in 30 ml. water to give 70.5% 2-nitro-4,6-dimethoxyphenyl-N-(p-dimethylaminophenyl)nitrone (IX), decomposed 175-7°. IX (4.5 g.) in 10 ml. AcOH was treated with 30% H2SO4 to give 91% 2,4,6-(O2N)(MeO)2C6H2CHO (X), m. 154-5°. A mixture of 844 mg. X, 1036 mg. 6-bromohomopiperonylic acid, 0.55 ml. Et3N, and 10 ml. Ac2O was heated 20 hrs. at 90-3° to give 54.6% 2-bromo-4,5-methylenedioxy-2'-nitro-4',6'-dimethoxy-cis-stilbene-α-carboxylic acid (XI), m. 268-70°; Me ester m. 161-2°. XI (986 mg.) in 25 ml. 5% NaOH was treated with 4.4 g. FeSO4 in 25 ml. water. The mixture was boiled 10 min. to give 85% 2-bromo-4,5-methylenedioxy-2'-amino-4',6'-dimethoxy-cis-stilbene-α-carboxylic acid (XII), m. 113-25°. A crude mixture of 760 mg. XII, 8 ml. HCONMe2, 8 ml. MeOH, and 8 ml. HCl-saturated MeOH was treated with 0.29 ml. iso-C5H11NO2. The diazonium salt was decomposed with 1 g. Cu (Natur Kupfer C) to give 42% 1,3-dimethoxy-5,6-methylenedioxy-8-bromophenanthrene-9-carboxylic acid

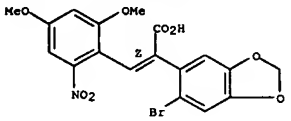
L4 ANSWER 215 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(XIII), decompd. 250-3°; Me ester m. 187-8.5°. Zn (4 g.) stirred in 4 g. H2O was treated with 30 mg. CuSO4 in 6 ml. water, followed by 338 mg. XIII and 10 ml. 10% KOH in MeOH. The mixt. was refluxed 1.5 hrs., followed by the addn. of 25 ml. 25% HCl and 5 g. Celite, to give after filtration 90.7% 1,3-dimethoxy-5,6-methylenedioxyphenanthrene-9-carboxylic acid (XIV), decompg. 300-3°. A mixt. of 31.5 mg. XIV, 300 mg. Cu, and 2 ml. quinoline was refluxed under N at 210-30° for 10 min. to give 69% III; picrate m. 175-7°. CH2N2 in 25 ml. Et2O was treated with 100 mg. XIV in 5 ml. HCONMe2 and 5 ml. MeOH to give 90% Me 1,3 - dimethoxy - 5,6 - methylenedioxyphenanthrene - 9 - carboxylate, m. 223-4°, which upon treatment with N2H4.H2O and MeOH gave 90% 1,3-dimethoxy-5,6-methylenedioxyphenanthrene-9-carboxylic acid hydrazide (XV), decompg. 246-50°. XV (47 mg.) in 5 ml. THF was treated with 5 ml. HCl-satd. MeOH and with 0.2 ml. iso-C5H11NO2 at 5° to give 86% 1,3 - dimethoxy - 5,6 - methylenedioxyphenanthrene - 9-carboxylic acid azide (XVI), m. 170-85°. A mixt. of 40 mg. XVI, 3 ml. Ac2O, and 0.25 ml. AcOH was heated under N 10 hrs. at 100° to give 78% IV, m. 294-5°.

IT 15994-97-5P 16136-21-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 15994-97-5 CAPLUS

CN Acrylic acid, 2-(2-bromo-4,5-(methylenedioxy)phenyl]-3-(2,4-dimethoxy-6-nitrophenyl)-, (Z)- (8CI) (CA INDEX NAME)

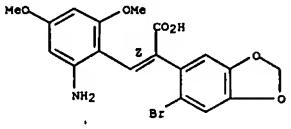
Double bond geometry as shown.



RN 16136-21-3 CAPLUS

CN Acrylic acid, 3-(2-amino-4,6-dimethoxyphenyl)-2-[2-bromo-4,5-(methylenedioxy)phenyl]-, (Z)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 215 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 216 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1967:37867 CAPLUS
DOCUMENT NUMBER: 66:37867
TITLE: Syntheses of pyridazine derivatives. X. Reactions of pyridazon-4-ylacetic acids
AUTHOR(S): Krbavcic, Alec; Tisler, Miha
CORPORATE SOURCE: Univ. Ljubljana, Ljubljana, Yugoslavia
SOURCE: Monatshefte fuer Chemie (1966), 97(5), 1494-8
CODEN: MOCHAP
DOCUMENT TYPE: Journal
LANGUAGE: German

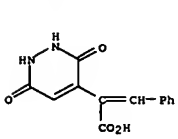
GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract 3-Hydroxy-6-(1H)-pyridazon-4-ylacetic acid (I) and its 1-Ph derivative (II) underwent condensation reactions typical of compds. with active methylene groups. I and BzH in Ac2O with Et3N gave 38% 3-phenyl-2-[3-hydroxy-6(1H)-pyridazon-4-yl]acrylic acid, m. 210° (decompn). I in aqueous NaOH with NaOAc and PhN2Cl yielded 25% 3-hydroxy-4-formyl-6(1H)-pyridazone phenylhydrazone, m. 165-70° (decomposition). II with the appropriate diazonium salts gave 32% phenylhydrazone, m. 280-2°, and 24% p-carboxyphenylhydrazone [m. 210-30° (decomposition)] of 1-phenyl-3-hydroxy-4-formyl-6(1H)-pyridazone. The Et ester of I and N2H4 hydrate in EtOH refluxed 0.5 hr. yielded 81% hydrazide, m. 320°, which with K2CO3 and CS2 in MeOH refluxed 6 hrs. gave 44% 5-[3-hydroxy-6(1H)-pyridazon-4-yl]-methyl-1,3,4-oxadiazoline-2(3H)-thione, III (R = H), m. 230-5°. 1-Phenyl-3-hydroxy-6(1H)-pyridazonyl-4-acetic acid hydrazide, m. 335-40°, prepared in 62% yield, heated 1 hr. at 150° with K2CO3 and CS2 in MeOH in an autoclave gave 56% III (R = Ph), m. >340°.

IT 13526-74-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13526-74-4 CAPLUS

CN 4-Pyridazineacetic acid, α-benzylidene-1,6-dihydro-3-hydroxy-6-oxo- (8CI) (CA INDEX NAME)



L4 ANSWER 217 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:93318 CAPLUS
DOCUMENT NUMBER: 64:93318
ORIGINAL REFERENCE NO.: 64:17538c-h,17539a
TITLE: 6-Quinolylacetic and 6-(1,2,3,4-tetrahydroquinolyl)acetic acid derivatives
AUTHOR(S): Bojarska-Dahlig, Halina
CORPORATE SOURCE: Inst. Farm., Warsaw
SOURCE: Roczniki Chemii (1965), 39(11), 1611-23
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

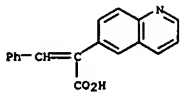
AB A series of the title compds. has been prepared as the potential monoamine oxidase (MAO) inhibitors. Thus, a mixture of 8.505 g. p-NH2C6H4CH2CO2H, 4.9 g. PhNO2, 2.14 g. FeSO4.5H2O, 3.65 g. H3BO3, 19 g. HOCH2CH(OH)CH2OH, and 10.7 ml. concentrated H2SO4 was refluxed 5 hrs., to give 6.6 g. 6-quinolylacetic acid (I), m. 215-18°; hydrochloride m. 216-18°; Me ester b13 196-200° n20D 1.5798 (picrate m. 137°); Et ester (II) b2.5 161-2°, m. 26-7°, n31.5D 1.5765 (picrate m. 136-8°); amide m. 209-9.5°; hydrazide (III), m. 163-4°; benzylamide m. 147-8° (hydrochloride m. 90-5°); amphetamide m. 125-5.5° (hydrochloride m. 148-50°). III (6.03 g.) in 15 ml. H2O was acidified with H2SO4 treated at 50° with the appropriate aldehyde, heated 1.5 hrs. at 100°, and neutralized with NaHCO3 to give 6-quinolylacetic acid hydrazones (IV). The following IV were prepared (R, m.p., and % yield given): Ph, 172-3°, 99.5 (V); 2-pyridyl, 67-9°, 90; 4-pyridyl, 70-3°, 93. Hydrogenation of 5.61 g. I in 80% MeOH with 10% Pd/C at 80° under 50 atmospheric during 3 hrs., afforded 3.72 g. VI (R1 = R2 = H, R3 = OH) (VII), m. 150-2°; Me ester b3 168-72°, n20D 1.5720 (picrate m. 141-3°); hydrazide m. 154-5°; benzylidenehydrazide m. 147-8° (VIII); benzylamide m. 126-7° (hydrochloride m. 130°); o-chlorobenzylamide m. 153-4° (hydrochloride m. 145°); amphetamide m. 115-16° (hydrochloride m. 124-6°). Hydrogenation of 21.5 g. II in EtOH either with 1.08 g. 10% Pd-C or 2.16 g. 5% Pd-Al2O3 at 80° under 50 atmospheric during 4 hrs. gave 19.6 g. Et ester (IX) of VII, b1.5 165-6°, n20D 1.5545; picrate m. 213° (dilute alc.). A solution of 7.25 g. VII, 6.13 g. NEt3, 4.59 g. ClCH2CN in 70 ml. EtOAc refluxed 3 hrs., gave a crude cyanomethyl ester separated as an oil which left with 30 ml. 30% NH4OH at 0° for 24 hrs., afforded 4.9 g. amide of VII, m. 170-3° (dilute alc.). Hydrogenation of 7.23 g. V in EtOH with 0.75 g. 10% Pd-C at 70° under 40 atmospheric during 3.5 hrs., gave 5.9 g. VI (R1 = R2 = H, R3 = NHNHCH2Ph) (X), m. 97-7.5°; hydrochloride m. 216-17°; tartrate m. 71-2°. Reduction of VIII carried out as described above yielded 86% X. A solution of 10.95 g. IX and 7.6 g. PhCH2Cl in 20 ml. PhMe refluxed 20 hrs. gave 9.1 g. VI (R1 = PhCH2, R2 = H, R3 = EtO) (XI), b5 230-1°, n20D 1.5838. Hydrolysis of 4.64 g. XI afforded 3.8 g. VI (R1 = PhCH2, R2 = H, R3 = OH), m. 95-6°; benzylamide m. 99-9.5°. IX (6.57 g.) and 4.19 g. 2-chloromethylpyridine in 15 ml. PhMe refluxed 20 hrs. gave 4.8 g. VI (R1 = 2-methylpyridyl, R2 = H, R3 = EtO) (XII), b0.3 190-3°; picrate m. 144-6°. Similarly prepared in 31% yield was VII [R1 = β-1-methyl-2-piperidyl)ethyl, R2 = H, R3 = EtO], b0.5 198-200°, n20D 1.5467; picrate m. 130-2°. Alkaline hydrolysis of XII yielded quant. VI (R1 = 2-methylpyridyl, R2 = H, R3

L4 ANSWER 217 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
= OH), m. 171°; benzylamide m. 55-7°. A mixt. of 16 g. Na salt of I, 8.1 g. PhCHO, 27.7 ml. Ac2O, and 2 drops pyridine was heated 20 hrs. at 150°, dild. with H2O, and steam distd. to remove BzH. The crude product pptd. with HCl and purified gave 16 g. α-(6-quinolyl)cinnamic acid, m. 255°; Et ester (XIII), b7 246-8°, m. 60-1°) picrate m. 215-16°). Hydrogenation of XIII, as described above for II, yielded 77% VII (R1 = H, R2 = PhCH2, R3 = EtO) (XIV), b6 257-60°, n20D 1.5812; picrate m. 116-18°. Alk. hydrolysis of XIV with aq. NaOH during 3.5 hrs. followed by acidification with HCl gave VII (R1 = HCl, R2 = PhCH2, R3 = OH), m. 166-8°. Benzylamide prepd. from XIV m. 102-4°. XIV refluxed with PhCH2Cl, as described for IX, yielded 59.6% VII (R1 = R2 = PhCH2, R3 = EtO) (XV), b2.5 265-9°, m. 73-3.5°. When refluxed with PhCH2NH2 XV yielded 53% VII (R1 = R2 = PhCH2, R3 = PhCH2NH), m. 112-15°.

IT 5622-70-8P, 6-Quinolineacetic acid, α-benzylidene-
RL: PREP (Preparation)
(preparation of)

RN 5622-70-8 CAPLUS

CN 6-Quinolineacetic acid, α-benzylidene- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 218 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:93300 CAPLUS
DOCUMENT NUMBER: 64:93300
ORIGINAL REFERENCE NO.: 64:17532d-h,17533a-e
TITLE: Preparation of cis-stilbazoles
AUTHOR(S): Galiazzo, Guido
CORPORATE SOURCE: Univ. Padua
SOURCE: Gazzetta Chimica Italiana (1965), 95(11), 1322-34
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Italian

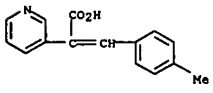
GI For diagram(s), see printed CA Issue.

AB The preparation of a series of cis-2-, -3-, and -4-styrylpyridine derivs. (I), with substituents in the benzene and pyridine rings, was described. The conversion of the trans derivs. (prepared according to Shaw, CA 27, 1630) was mainly made by uv irradiation, according to one of the following methods: (A) trans-3,4'-Dimethyl-4-stilbazole (10 g.) was treated with 10 cc. 36% HCl in 1500 cc. H2O, stirred, and irradiated during 50 hrs. with a 1000-w. Hg lamp, fixed at a distance of 15-20 cm., the liquid offering a surface of 25 cm. diameter and the concentration being kept constant by the addition of H2O; after addition of NH3, the solution was extracted with C6H6, the extract dried over Na2SO4, the solvent evaporated in vacuo, the residue taken up in 150 cc. n-heptane, the solution filtered, the filtrate evaporated, the process repeated with 100 cc. petr. ether, and the residue distilled at 120°/0.1 mm. to give 5 g. of a green liquid, which was further purified by passing its solution in petr. ether and then in C6H6, through an alumina column, the characterization of the last fraction being made by uv and ir spectra. (B) A solution of 5 g. 4'-methoxy-4-stilbazole in 120 cc. C6H6 was irradiated, with simultaneous stirring and cooling, by means of a low pressure 1000-w. immersion lamp, during 40 hrs.; the solvent was evaporated in vacuo, the residue taken up in boiling n-heptane to give, after cooling, 2.1 g. trans derivative which was filtered off, the filtrate evaporated to dryness, the process repeated with petr. ether, and the residue worked up as above. (C) A solution of 5 g. trans-3-methyl-2-stilbazole (trans-II) in 150 cc. C6H6 was filled in a 200-cc. ampul, the air replaced by N, and the sealed ampul irradiated during 350 hrs. with a high-pressure 1000-w. Hg lamp; the solution was worked up as above. The same procedure was applied to a solution of 5 g. trans-II in 240 cc. H2O and 8 cc. 36% HCl; working up consisted in neutralizing with Na2CO3, extracted with C6H6, and concentrating the solution to give 3 g. of the dimer of trans-II, m. 173°. Repeated extns. of the filtrate with petr. ether gave finally 0.6 g. cis-II (see 1st table). A solution of 41 g. phenyl(4-pyridyl)acetylene [prepared from 4-stilbazole (III) by bromination and treatment with KOH] in 500 cc. EtOH was reduced over 0.8 g. 5% Pd on CaCO3 to give 27 g. cis-III b0.5 100-5°. Starting from the following phenylpyridylacrylic acids (IV) some cis and trans derivs. of 3-stilbazole (V) were prepd. by the Perkin synthesis (2nd table): α-phenyl-β-(3-pyridyl)acrylic acid, m. 197-200°; α-(4-chlorophenyl)-β-(3-pyridyl)acrylic acid, m. 220°; α-(4-bromophenyl)-β-(3-pyridyl)acrylic acid, m. 183°; α-(4-iodophenyl)-β-(3-pyridyl)acrylic acid (IVa), m. 189-95°; α-(3-pyridyl)-β-(4-methylphenyl)acrylic acid, m. 198°; α-(3-pyridyl)-β-(4-methoxyphenyl)acrylic acid, m. 230°. R1, R2, R3, b.p./0.1 mm., m.p.; cis, , , , ; 3-pyridyl, H, H, 105°, --; 3-pyridyl, H, Me, 120°, --; 3-pyridyl, H, Cl, 115°, --; 3-pyridyl, H, Br, 125°, --; 3-pyridyl, H, I (cis-Va), 140°, --; 3-pyridyl, H, MeO, 125°, --; 3-pyridyl, H, NO2, 135°, 54°; trans, , , , ; H, 3-pyridyl, H, --, 78°; H, 3-pyridyl, Me, --, 111°; H, 3-pyridyl, Cl, --, 87°; H, 3-pyridyl, Br, --, 101°; H, 3-pyridyl, I (trans-Va), --, 153°; H, 3-pyridyl, MeO, --, 103°; H, 3-pyridyl, NO2, --, 153°; Thus, nitration of 150 g. PhCH2CN gave 110 g. p-O2NC6H4CH2CN, m. 116-17°, hydrolysis of which by refluxing with 1:1 aq. H2SO4 for 15-20 min. gave 115 g. p-O2NC6H4CH2CO2H, m. 155°. This was dissolved in 575 cc. 6N NH3 and treated with H2S at 35° to give 73.7 g. p- H2NC6H4CH2CO2H, m. 202-3°; 52 g. of this compd. was dissolved in 100 cc. AcOH, 140 cc. concd. H2SO4, and 2000 cc. H2O, and diazotized with 23.7 g. NaNO2 at 0°; after removal of HNO2, 120 g. KI was added, the mixt. kept 24 hrs. at room temp., heated on a water bath, treated with C, and filtered hot to give 28 g. p-IC6H4CH2CO2H, m. 138°. This compd. was dissolved in 250 cc. EtOH, treated with 4.4 g. NaOH, refluxed, the solvent evapd. in vacuo, 12 g. 3-pyridinecarboxaldehyde and 56 g. Ac2O added, and the mixt. refluxed 2 hrs. to give 35 g. IVa. Decarboxylation of IVa was accomplished by addn. in small portions to a boiling soln. of 5.25 g. Cu chromite in 70 cc. quinoline, refluxing the mixt. 20 min., decanting the formed CuCrO2, evapg. the solvent in vacuo at 65-70°/0.5 mm., and collecting cis-Va as a first fraction in 59% yield; the 2nd fraction (8 g.), b. >140°, was dissolved in 300 cc. n-heptane, a few cc. satd. iodine soln. in the same solvent added, and the mixt. irradiated during 5 hrs. with a tungsten lamp to give quant. trans-Va.

IT 5847-78-9P, 3-Pyridineacetic acid, α-(p-methylbenzylidene)-
5847-83-6P, 3-Pyridineacetic acid, α-(p-methoxybenzylidene)-
RL: PREP (Preparation)
(preparation of)

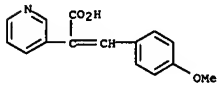
RN 5847-78-9 CAPLUS

CN 3-Pyridineacetic acid, α-(p-methylbenzylidene)- (7CI, 8CI) (CA INDEX NAME)



RN 5847-83-6 CAPLUS

CN 3-Pyridineacetic acid, α-[(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

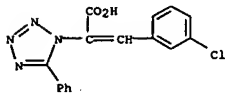


L4 ANSWER 219 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:431661 CAPLUS
DOCUMENT NUMBER: 63:31661
ORIGINAL REFERENCE NO.: 63:5631b-c
TITLE: The azidolysis of 4-arylidene- and 4-alkylidene-5-oxazolones
AUTHOR(S): Awad, W. I.; Fahmy, A. F. M.; Sammour, A. M. A.
CORPORATE SOURCE: Ain Shams Univ., Cairo
SOURCE: Journal of Organic Chemistry (1965), 30(7), 2222-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Tetrazolylcinnamic acid derivatives are prepared by a simple method in good yields. Infrared spectra of these acids reveal two types of acids in the solid state: (a) a dipolar type in equilibrium with its monomer, and (b) normal bonded acids. The ultraviolet spectra show that the methyl group in the 5-position has no interaction with the tetrazolyl ring while a phenyl group has. Under similar conditions 4-isopropylidene- and 4-cyclohexylidene-5-oxazolones gave no tetrazolylacrylic acid derivatives and the reaction proceeds via another route with decarbonylation to give iso-PrCONHCOPh, iso-PrCONHCOC6H4Cl-p, and C6H11CONHCOPh. The constitution of these products is discussed in the light of their uv, ir, and N.M.R. spectra.

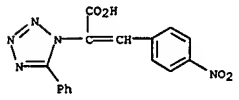
IT 1738-44-9P, 1H-Tetrazole-1-acetic acid, α-(m-chlorobenzylidene)-5-phenyl- 1738-45-0P, 1H-Tetrazole-1-acetic acid, α-(p-nitrobenzylidene)-5-phenyl- 1738-46-1P, 1H-Tetrazole-1-acetic acid, α-(m-nitrobenzylidene)-5-phenyl- 1738-47-2P, 1H-Tetrazole-1-acetic acid, α-(o-nitrobenzylidene)-5-phenyl- 1738-48-3P, 1H-Tetrazole-1-acetic acid, α-(p-methoxybenzylidene)-5-phenyl- 1738-50-7P, 1H-Tetrazole-1-acetic acid, α-benzylidene-5-methyl- 1738-51-8P, 1H-Tetrazole-1-acetic acid, α-(p-chlorobenzylidene)-5-methyl- 1738-52-9P, 1H-Tetrazole-1-acetic acid, 5-methyl-α-(m-nitrobenzylidene)- 1738-53-0P, 1H-Tetrazole-1-acetic acid, α-(p-methoxybenzylidene)-5-methyl- 1738-65-4P, 1H-Tetrazole-1-acetic acid, α-benzylidene-5-phenyl- 1738-66-5P, 1H-Tetrazole-1-acetic acid, α-(p-chlorobenzylidene)-5-phenyl- 1964-79-0P, 1H-Tetrazole-1-acetic acid, α-(o-chlorobenzylidene)-5-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 1738-44-9 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(m-chlorobenzylidene)-5-phenyl- (7CI, 8CI) (CA INDEX NAME)

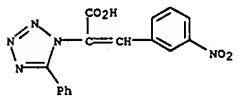


L4 ANSWER 219 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

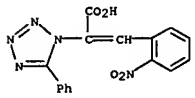
RN 1738-45-0 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[(4-nitrophenyl)methylene]-5-phenyl- (9CI) (CA INDEX NAME)



RN 1738-46-1 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(m-nitrobenzylidene)-5-phenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

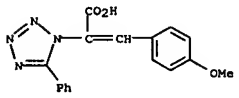


RN 1738-47-2 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(o-nitrobenzylidene)-5-phenyl- (7CI, 8CI) (CA INDEX NAME)

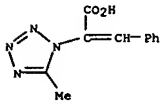


RN 1738-48-3 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-methoxybenzylidene)-5-phenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

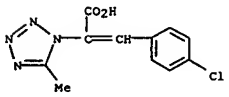
L4 ANSWER 219 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



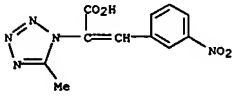
RN 1738-50-7 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 1738-51-8 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-chlorobenzylidene)-5-methyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

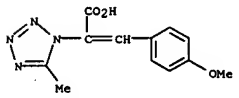


RN 1738-52-9 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-methyl-α-(m-nitrobenzylidene)- (7CI, 8CI) (CA INDEX NAME)

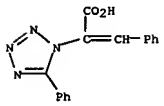


RN 1738-53-0 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-methoxybenzylidene)-5-methyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

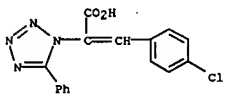
L4 ANSWER 219 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



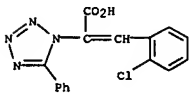
RN 1738-65-4 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-phenyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 1738-66-5 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-chlorobenzylidene)-5-phenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)



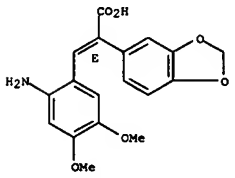
RN 1964-79-0 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(o-chlorobenzylidene)- (8CI) (CA INDEX NAME)



L4 ANSWER 220 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:461794 CAPLUS
DOCUMENT NUMBER: 59:61794
ORIGINAL REFERENCE NO.: 59:11317a-c
TITLE: α-(3,4-Methylenedioxyphenyl)-2-nitro-4,5-dimethoxycinnamic acid
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi; Hiraoka, Hisanao; Honda, Hiroshi
CORPORATE SOURCE: Nagoya City Univ., Japan
SOURCE: Nagoya-shiritsu Daigaku Yakugakubu Kiyo (1962), 10, 54-6
CODEN: NADYAS; ISSN: 0469-4805
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB A mixture of 1.8 g. 3,4-methylenedioxyphenylacetic acid, 2.1 g. 2-nitro-4,5-dimethoxybenzaldehyde, 4 cc. Ac2O, and 2 cc. Et3N is refluxed at 100° for 20 hrs., 2 cc. H2O added, a solution of 16 g. K2CO3 in 100 cc. H2O added, and the mixture washed with Et2O, and acidified with concentrated HCl. The precipitate (1.5 g.) is dissolved in 200 cc. 2% NH4OH, filtered, and the filtrate acidified with AcOH to precipitate 1.1 g. trans-α-(3,4-methylenedioxyphenyl)-2-nitro-4,5-dimethoxycinnamic acid (I), yellow columns, m. 197-7.5°. The mother liquor is made strongly acid with concentrated HCl to give 0.2 g. corresponding cis compound (II), yellow needles, m. 214-15° (C6H6). To 3 cc. aqueous solution of 1.5 g. FeSO4.7H2O is added 3.5 cc. NH4OH, a solution of 0.25 g. I in 5 cc. 5% NH4OH added, the mixture agitated 20 min., filtered, and the filtrate neutralized with HCl to give 0.18 g. 3-(3,4-methylenedioxyphenyl)-6,7-dimethoxycarbostyril (III), needles, m. 328-9° (decomposition) (EtOH). Refluxing of II in EtOH for 12 hrs. also gives III. trans-α-(3,4-Methylenedioxyphenyl)-2-amino-4,5-dimethoxycinnamic acid, yellow needles, m. 228-30° (decomposition), is made from II.
IT 875537-13-6P, Acrylic acid, 3-(2-amino-4,5-dimethoxyphenyl)-2-[3,4-(methylenedioxy)phenyl]-, trans- 875611-22-6P, Acrylic acid, 3-(4,5-dimethoxy-2-nitrophenyl)-2-[3,4-(methylenedioxy)phenyl]-, trans-
RL: PREP (Preparation)
(preparation of)
RN 875537-13-6 CAPLUS
CN Acrylic acid, 3-(2-amino-4,5-dimethoxyphenyl)-2-[3,4-(methylenedioxy)phenyl]-, trans- (7CI) (CA INDEX NAME)

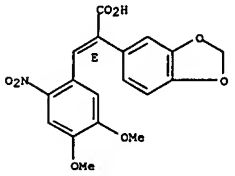
Double bond geometry as shown.

L4 ANSWER 220 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

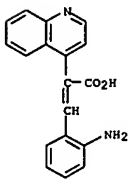


RN 875611-22-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



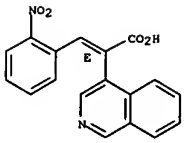
L4 ANSWER 221 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:448258 CAPLUS
DOCUMENT NUMBER: 59:48258
ORIGINAL REFERENCE NO.: 59:8700g-h,8701a
TITLE: A new synthetic approach to the benzo[c]phenanthridine system: internuclear cyclization onto a pyridine ring
AUTHOR(S): Abramovitch, R. A.; Tertzakian, G.
CORPORATE SOURCE: Univ. Saskatchewan, Saskatoon
SOURCE: Canadian Journal of Chemistry (1963), 41(9), 2265-71
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Benzo[c]phenanthridine (I) has been synthesized in low overall yield by the Pschorr cyclization of trans-α-(4-isoquinolyl)-o-aminocinnamic acid. The condensation of 4-isoquinolylacetonitrile with o-nitrobenzaldehyde gave the cis-cinnamonitrile. The preparation of a number of intermediates is described.
IT 94331-05-2P, 4-Quinolineacetic acid, α-(o-aminobenzylidene)-, trans- 875540-35-5P, 4-Isoquinolineacetic acid, α-(o-nitrobenzylidene)-, trans-
RL: PREP (Preparation)
(preparation of)
RN 94331-05-2 CAPLUS
CN 4-Quinolineacetic acid, α-(o-aminobenzylidene)- (7CI) (CA INDEX NAME)



RN 875540-35-5 CAPLUS
CN 4-Isoquinolineacetic acid, α-(o-nitrobenzylidene)-, trans- (7CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 221 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



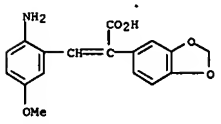
L4 ANSWER 222 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:81625 CAPLUS
DOCUMENT NUMBER: 55:81625
ORIGINAL REFERENCE NO.: 55:15441h-i,15442a-f
TITLE: Phenanthrene derivatives. III. Synthesis of 2-methoxy-5,6-methylenedioxyphenanthrene and 2-methoxy-6,7-methylenedioxyphenanthrene
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi
CORPORATE SOURCE: Nagoya City Univ.
SOURCE: Chemical & Pharmaceutical Bulletin (1960), 8, 727-31
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 53, 13123d. Condensation of 6 g. 3,4-(CH2O2)C6H3CH2CO2Na (I) with 5.4 g. 2,5-(O2N)(MeO)C6H3CHO (II) by heating 7 hrs. at 110° in 30 cc. Ac2O yielded 4.1 g. trans-2,5-(O2N)(MeO)C6H3CH:CRCO2H (R = 3,4-CH2O2C6H3) (III), m. 175°, and from the mother liquor 0.03 g. cis isomer (IV), m. 188-9°, with a trace of trans-2,5-(O2N)(MeO)C6H3CH:CHCO2H, m. 229°. III (1.4 g.) reduced with FeSO4.7H2O in NH4OH yielded 1.1 g. corresponding aminocinnamic acid (V), m. 248° (decomposition), whereas 0.05 g. IV similarly reduced was cyclized to yield 0.03 g. 3-(3,4-methylenedioxyphenyl)-6-methoxycarbostyril (VI), m. 280-2° (decomposition), formed also (0.06 g.) by refluxing 0.1 g. V 10 hrs. in 10 cc. absolute EtOH. For ring closure of V to the desired phenanthrene derivative, the Pschorr reaction was applied.
Diazotization of 1 g. V in MeOH, followed as usual by addition of Gattermann Cu yielded unexpectedly 0.3 g. 2,2'-hydrazobis[α-(3,4-methylenedioxyphenyl)-5-methoxycinnamic acid] (VII), m. 226° (decomposition). The structure of VII was confirmed by both ultraviolet and infrared absorption spectra, and by its catalytic hydrogenation (0.1 g.) in EtOH (Pd-C) to give 0.06 g. 3-(3,4-methylenedioxyphenyl)-6-methoxy-3,4-dihydrocarbostyril, m. 202°, identical by mixed m.p. with the product (0.22 g.) from similar catalytic hydrogenation of 0.34 g. III. However, 1 g. V diazotized as before, but 0.5 g. NaH2PO4 added before addition of Gattermann Cu yielded 0.24 g. 2-methoxy-6,7-methylenedioxy-9-phenanthrenecarboxylic acid (VIII), m. 237-8° (decomposition), with a trace of trans-2,5-H2N(MeO)C6H4CH:CRCO2H (R = 3,4-CH2O2C6H3), m. 203-4°, identical by mixed m.p. with an authentic sample prepared according to Kostanecki and Sulser [Ber. 38, 941(1905)]. Decarboxylation of 0.2g. VIII by boiling with powdered Cu in quinoline, followed by Al2O3 chromatography yielded 0.02 g. of the desired 2-methoxy-6,7-methylenedioxyphenanthrene (IX), m. 178°; picrate, m. 139-41° (decomposition). The 6,7-position of the CH2O2 group was established by synthesis of the quite different isomeric 2-methoxy-5,6-methylenedioxyphenanthrene (X). II (0.9 g.) condensed with 1.4 g. 6-bromo derivative of I yielded 0.9 g. trans-2,5-(O2N)(MeO)C6H3CH:CRCO2H [R = 2,4,5-Br(CH2O)2C6H2], m. 198-9°, and this (1 g.) reduced (as was III) with FeSO4.7H2O in NH4OH yielded 0.8 g. corresponding aminocinnamic acid (XI), m. 229-30° (decomposition). XI (0.1 g.) refluxed 10 hrs. in EtOH (as was V) yielded 0.06 g. 3-(2-bromo-4,5-methylenedioxyphenyl)-6-methoxycarbostyril, m. 265°.

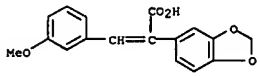
L4 ANSWER 222 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Diazotization of 0.5 g. XI, followed by addn. of Gattermann Cu yielded 0.2 g. 1-bromo-3,4-methylenedioxy-7-methoxy-10-phenanthrenecarboxylic acid, which (0.1 g.) without purification was dehalogenated by refluxing 24 hrs. with Zn in NaOH to yield 0.04 g. 2-methoxy-5,6-methylenedioxy-9-phenanthrenecarboxylic acid, m. 232-5°, and this (0.04 g.) finally was decarboxylated (as was VIII) to yield 0.01 g. X, m. 130-1°; picrate, m. 140-1° (decompn.). Ultraviolet absorption data were reported for III-X.

IT 110394-32-6P, Acrylic acid, 3-(2-amino-5-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- 110423-68-2P, Acrylic acid, 3-(m-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- 111141-34-5P, Acrylic acid, 3-(2-amino-5-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- 130862-00-9P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(5-methoxy-2-nitrophenyl)-, trans- 857175-97-4P, Acrylic acid, 3,3'-[azobis(5-methoxy-o-phenylene)]bis[2-(3,4-methylenedioxyphenyl)- 876659-62-0P, Acrylic acid, 3-(5-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- 876659-63-1P, Acrylic acid, 3-(5-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, cis-
RL: PREP (Preparation)
(preparation of)

RN 110394-32-6 CAPLUS
CN Acrylic acid, 3-(2-amino-5-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)-(6CI) (CA INDEX NAME)

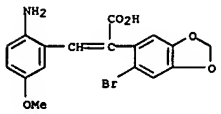


RN 110423-68-2 CAPLUS
CN Acrylic acid, 3-(m-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



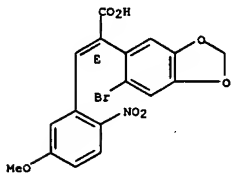
RN 111141-34-5 CAPLUS
CN Acrylic acid, 3-(2-amino-5-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)

L4 ANSWER 222 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

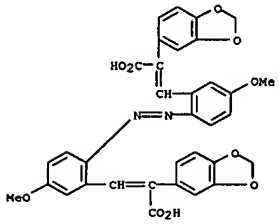


RN 130862-00-9 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(5-methoxy-2-nitrophenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



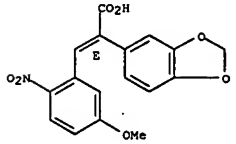
RN 857175-97-4 CAPLUS
CN Acrylic acid, 3,3'-[azobis(5-methoxy-o-phenylene)]bis[2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 876659-62-0 CAPLUS
CN Acrylic acid, 3-(5-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

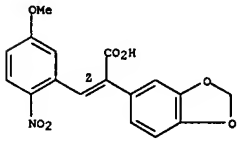
Double bond geometry as shown.

L4 ANSWER 222 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



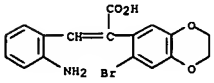
RN 876659-63-1 CAPLUS
CN Acrylic acid, 3-(5-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, cis- (6CI) (CA INDEX NAME)

Double bond geometry as shown.

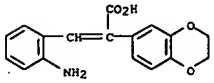


L4 ANSWER 223 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:54305 CAPLUS
DOCUMENT NUMBER: 55:54305
ORIGINAL REFERENCE NO.: 55:10449d-i,10450a
TITLE: Synthesis in the morphinan group. IV. Structural proof
of 2,3- and 3,4-ethylenedioxy-N-methylmorphinan
AUTHOR(S): Sasamoto, Mitsuo
CORPORATE SOURCE: Tanabe Seiyaku Co., Tokyo
SOURCE: Chemical & Pharmaceutical Bulletin (1960), 8, 329-35
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The title compds. (I and II, resp.) were subjected to the Hofmann degradation; by syntheses of their degradation products, their structures were confirmed. Thus, warming the MeI salts of I and II separately 12 hrs. at 50° with Ag2O gave the methohydroxides, which (heated 1.5 hrs. at 120°) yielded from the C6H6 exts. 93.5% and 87.1%, resp., R' (III) and R (IV) derivs. of 13-(2-dimethylaminoethyl)-5,6,7,8,13,14-hexahydrophenanthrene; H oxalates m. 197-8° (decomposition) and 171-3° (decomposition), resp. Aromatization of III and IV was effected by heating them 6 hrs. with 10% Pd-C at 320° under N to yield 48% and 17%, resp., R' (V) and R derivs. (VI) of phenanthrene, m. 113-14° and 77.5-9.0°; picrates m. 175-6° and 150-1°, resp. Ultraviolet data for III-VI confirmed these structures of the Hofmann degradation products, which were further confirmed by their synthesis. The Perkin condensation of RC6H3CH2CO2Na with 2-O2NC6H4CHO in the presence of Ac2O in the usual way yielded 61.7% 2-O2NC6H4CH:C(CO2H)C6H3R, m. 195-7°, which was reduced to the corresponding 2-H2N compound (VII), m. 183°, by warming with FeSO4 in NH4OH. The Pschorr condensation of VII through diazotization with HNO2, and treatment of the diazonium salt with H2SO4 and Cu eliminated N and closed the ring to yield 8.2% and 3.1% 10-HO2C derivative of V and VI, resp., m. 272-4° and 241-3°, decarboxylated by treatment with Gattermann Cu in quinoline under N to 59.3% and 53% V and VI, resp., identical with the preceding samples and giving picrates identical with those above. The ultraviolet and infrared curves of the 2 samples of V and of VI were superimposable. For further confirmation that VI was the R
(and not the R') derivative of phenanthrene, it was synthesized independently.
RC6H3CHO brominated as usual with Br in AcOH yielded 15.7% 6-Br derivative
(VIII), m. 149-50°, formed also (13.1%) from 6,3,4-Br(HO)2C6H2CHO refluxed 44 hrs. on a water bath with (CH2Br)2 and NaOH in EtOH. Heating VIII (as was III in the preceding part) with hippuric acid, anhydrous AcONa,
and Ac2O yielded 66% 6-Br derivative of RC6H3CH:C.C(O).O.CPh:N, m. 263-4°, which was converted to 37% 6-Br derivative of V of the preceding part, b2 150-2°. This was hydrolyzed to 84% corresponding acid, m. 219-20°, whose Na salt condensed with 2-O2NC6H4CHO yielded 65.1% 2-nitro-α-(2-bromo-4,5-ethylenedioxyphenyl)cinnamic acid, m. 216-17°, and this was reduced with FeSO4 in NH4OH to 74% corresponding H2N compound (IX), m. 125-8°

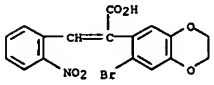
L4 ANSWER 223 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



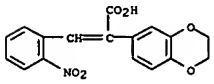
L4 ANSWER 223 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(decompn.). IX was subjected to the Pschorr condensation (as was VII) to yield 10.5% 1,10-Br(HO2C) deriv. of VI, m. 256-8° (decompn.), and this debrominated with Zn-Cu couple gave the 10-HO2C deriv. of VI, identical with the sample formed above.
IT 101442-55-1P, 1,4-Benzodioxan-6-acetic acid, α-(o-aminobenzylidene)- 101576-01-6P, 1,4-Benzodioxan-6-acetic acid, 7-bromo-α-o-nitrobenzylidene- 101601-19-8P, 1,4-Benzodioxan-6-acetic acid, α-o-nitrobenzylidene- 101602-10-2P, 1,4-Benzodioxan-6-acetic acid, α-(o-aminobenzylidene)-7-bromo-
RL: PREP (Preparation)
(preparation of)
RN 101442-55-1 CAPLUS
CN 1,4-Benzodioxan-6-acetic acid, α-(o-aminobenzylidene)- (6CI) (CA INDEX NAME)



RN 101576-01-6 CAPLUS
CN 1,4-Benzodioxan-6-acetic acid, 7-bromo-α-o-nitrobenzylidene- (6CI) (CA INDEX NAME)



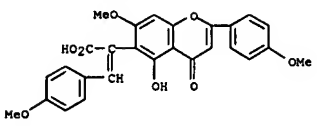
RN 101601-19-8 CAPLUS
CN 1,4-Benzodioxan-6-acetic acid, α-o-nitrobenzylidene- (6CI) (CA INDEX NAME)



RN 101602-10-2 CAPLUS
CN 1,4-Benzodioxan-6-acetic acid, α-(o-aminobenzylidene)-7-bromo- (6CI) (CA INDEX NAME)

L4 ANSWER 224 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:17917 CAPLUS
DOCUMENT NUMBER: 55:17917
ORIGINAL REFERENCE NO.: 55:3579a-f
TITLE: The structure of ginkgetin. V. Flavone carboxylic acid
AUTHOR(S): Kogure, Akira
CORPORATE SOURCE: Osaka City Univ.
SOURCE: Nippon Kagaku Zasshi (1959), 80, 1462-6
CODEN: NPKZAZ; ISSN: 0369-5387
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB A flavonecarboxylic acid, C25H2009 (I), was obtained from ginkgetin (Ia) by treating with KOH-H2O, which gave the Me ether Me ester (II) with CH2N2
(cf. preceding abstract). II showed pos. FeCl3 reaction, λ 2.71, 3.21, 5.8, 6.00 μ, suggesting the existence of still more hydroxy groups. II heated with Ac2O and AcONa gave the two acetates, C30H2608, m.
139-141°, and C32H30011, m. 196-8°. II gave the carboxylic acid Me ether (III), C27H2409, pale yellow, insol. in NaHCO3 solution III gave C27H2208, m. 216-18°, yellow, supposedly a dehydrated III, by boiling with MeOH-HCl. I with alc. H2SO4 gave the Me ester, C27H2409, yellow, m. 188-190°, reconverted to I by hydrolysis and converted to the Me ether, m. 220-2°, by CH2N2, then further to III by hydrolysis. I gave the acetate, C33H28013, m. 222-4°, by acetylation and the Me ether Me ester (IV), C30H3009, m. 221-2°, different from II, with Me2SO4. IV had no carbonyl group other than one in the γ-pyrone ring, since IV did not form the oxime under mild conditions. IV was hydrolyzed to a flavonecarboxylic acid Me ether (V), C29H2809, m. 298°, converted to the Et ester, C31H3209, m. 208-210°, by treating with alc. HCl. In an attempt to decarboxylate by boiling with quinoline and Cu, IV was recovered unchanged
or decomposed, indicating that the carboxy group in IV was not attached to
the double bond. Heating V at 305° 7-8 min. gave the flavone lactone (VI), C27H2208, m. 215-16°, by demethylation and dehydration, green with FeCl3. VI yielded the acetate, C29H2409, m. 185-7°. Hydrolysis of VI with 5% alc. KOH gave a flavonecarboxylic acid (VII), C27H2409, m. 298-300°. IV was prepared by methylation of VII with MeI or from VI with Me2SO4. These results showed that I was not easily decarboxylated but lactonized quickly. On ozonization, Ia di-Me ether gave a flavonecarboxylic acid Me ether (VIII), m. 297-8°. VIII kept at 305° 5-7 min. gave the lactonic flavone (IX), C26H2008, m. 225-6°, reconverted to VIII by treating with KOH or acetylated to C30H2010, m. 135°. Both VIII and IX yielded IV with Me2SO4. Ia with H2O2 in alkaline solution gave I rather than oxoflavone (part
IV). Demethyl derivative of Ia, m. above 320°, gave demethyl derivative of
I, which yielded IV with MeSO4. The structure of Ia was supposed to be a flavone nuclearly fused with a hydroflavonol.
IT 103210-81-7P, 4H-1-Benzopyran-6-acetic acid, 5-hydroxy-7-methoxy-α-p-methoxybenzylidene-2-(p-methoxyphenyl)-4-oxo-
RL: PREP (Preparation)
(preparation of)
RN 103210-81-7 CAPLUS
CN 4H-1-Benzopyran-6-acetic acid, 5-hydroxy-7-methoxy-α-p-methoxybenzylidene-2-(p-methoxyphenyl)-4-oxo- (6CI) (CA INDEX NAME)

L4 ANSWER 224 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 225 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

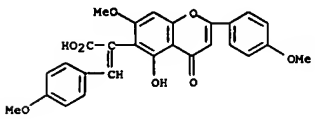
ACCESSION NUMBER: 1961:17916 CAPLUS
DOCUMENT NUMBER: 55:17916
ORIGINAL REFERENCE NO.: 55:3578i,3579a-b
TITLE: The structure of ginkgetin. IV. Alkali cleavage of ginkgetin
AUTHOR(S): Kogure, Akira
CORPORATE SOURCE: Osaka City Univ.
SOURCE: Nippon Kagaku Zasshi (1959), 80, 1355-8
CODEN: NPKZAZ; ISSN: 0369-5387
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Ginkgetin (I) boiled 40 min. in 30% aqueous KOH solution gave p-methoxyacetophenone (II), anisic acid (III), flavonecarboxylic acid (IV), C25H29O9, m. 308-10°, and oxoflavone (V), m. 269° (decomposition). I boiled in 40% aqueous KOH solution many hrs. gave acetic acid, II, III, and phloroglucinol. IV, C25H20O9, brown with FeCl3, red with HCl-Mg, was converted to the Me ether Me ester, C28H26O9, m. 214-15°, brown with FeCl3. V gave the oxime, m. 275-6°, and the semicarbazone, m. 228-30°. V gave the mono-Me ether, C27H22O7, m. 220-2°, green with FeCl3, converted to the acetate, C29H24O9, m. 224-6.5°. IV and V exibited ultraviolet absorption essentially identical with that of I.

IT 103210-81-7P, 4H-1-Benzopyran-6-acetic acid, 5-hydroxy-7-methoxy-α-p-methoxybenzylidene-2-(p-methoxyphenyl)-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 103210-81-7 CAPLUS

CN 4H-1-Benzopyran-6-acetic acid, 5-hydroxy-7-methoxy-α-p-methoxybenzylidene-2-(p-methoxyphenyl)-4-oxo- (6CI) (CA INDEX NAME)



L4 ANSWER 226 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

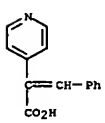
ACCESSION NUMBER: 1960:110527 CAPLUS
DOCUMENT NUMBER: 54:110527
ORIGINAL REFERENCE NO.: 54:21079h-i,21080a-c
TITLE: Antitubercular compounds. XVIII. Synthesis of a vinylog of isonicotinic acid hydrazine
AUTHOR(S): Kakimoto, Shichiro; Nishie, Jun; Yamamoto, Kenichi
CORPORATE SOURCE: Hokkaido Univ., Sapporo
SOURCE: Japan. J. Tuberc. (1959), 7, 76-80
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 53, 1552f; 54, 7694g. β-(4-Pyridyl)acrylic acid (1 g., prepared by condensing γ-picoline and CCl3CHO in AcOAm and hydrolyzing with alc. KOH), 0.68 g. Et3N, and 40 ml. CH2Cl2 refluxed 2 hrs., 0.73 g. ClCO2Et added with stirring at 0°, 2 ml. 80% N2H4.H2O added after 2 min., the cooled mixture stirred 30 min., the solvent distilled, the residue dissolved in EtOH, and the filtrate evaporated in vacuo gave 0.3 g. β-(4-pyridyl)acrylic acid hydrazide (I), needles, m. 109-10° (CH2Cl2). I (0.2 g.), 20 ml. EtOH, and 50 mg. PtO2 shaken at room temperature under 1 atmospheric H until 1 mole H was absorbed and the filtrate evaporated in vacuo yielded 0.15 g. β(4-pyridyl)propionic acid hydrazide (II), needles, m. 64° (CH2Cl2), containing 1 mole H2O of crystallization (dried crystals m. 84°). Et 4-pyridylacetate (1.8 g.), 2 g. PhCHO, and 10 ml. Ac2O refluxed 5 hrs. at 150-60°, the solvent distilled, the residue treated with aqueous K2CO3 and extracted with CHCl3, the residue from distillation of solvent (1.3 g. b3 180°) hydrolyzed 1 hr. with boiling 2N MeOH-KOH, the acid extracted with Et2O, the Et2O distilled, and the residue precipitated by HOAc from alkaline solution yielded 1 g. α-(4-pyridyl)cinnamic acid, decomposing 203° (EtOH). The acid (1 g.) gave 0.2 g. α-(4-pyridyl)cinnamic acid hydrazide (III), needles, m. 109-10°, by the method used in the preparation of I. Hydrogenation of III, as in the preparation of II, gave α-(4-pyridyl)dihydrocinnamic acid hydrazide (IV), needles, m. 138° (CH2Cl2). Ultraviolet spectra of I-IV and of 4-pyridylacetic acid hydrazide (V) were determined I and II showed bands in the infrared at 1659, 1625, and 1601 and at 1649 and 1607 cm.-1, resp. I showed in vitro antitubercular activity, but the other compds. (II-V) were inactive.

IT 106837-54-1P, 4-Pyridineacetic acid, α-benzylidene-
RL: PREP (Preparation)
(preparation of)

RN 106837-54-1 CAPLUS

CN 4-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



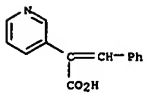
L4 ANSWER 226 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 227 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:44647 CAPLUS
DOCUMENT NUMBER: 54:44647
ORIGINAL REFERENCE NO.: 54:8813g-h
TITLE: 3-Styrylpyridine
AUTHOR(S): Beard, J. A. T.; Katritzky, A. R.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la Belgique (1959), 78, 592
CODEN: RTCPB4; ISSN: 0370-7539
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

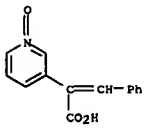
AB 3-Pyridylacetic acid (6.3 g.), 8 g. B2H, 50 ml. C5H5N, and 1 ml. piperidine were heated 72 hrs. at 120°, 3 g. NaOH in 150 ml. H2O added, the whole steam distilled, (HOAc) and the residue acidified to give
5.9 g. β-phenyl-α-3-pyridylacrylic acid (I), m. 235-6°.
I (0.5 g.) was heated 1 hr. at 250° with 15 ml. liquid paraffin.
After cooling, 40 ml. of ether was added, the mixture extracted with 20 ml. 2N
HCl, and the acid extract basified and extracted with Et2O to give 0.05 g. title
compound, m. 72-3°. The infrared showed it to be trans. I and aqueous peracetic acid gave 63% 1-oxide, m. 219-221°. This did not decarboxylate smoothly on pyrolysis.

IT 32967-19-4P, 3-Pyridineacetic acid, α-benzylidene-
100725-77-7P, 3-Pyridineacetic acid, α-benzylidene-, 1-oxide
RL: PREP (Preparation)
(preparation of)

RN 32967-19-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 100725-77-7 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)-, 1-oxide (9CI) (CA INDEX NAME)



L4 ANSWER 227 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 228 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:44595 CAPLUS
DOCUMENT NUMBER: 54:44595
ORIGINAL REFERENCE NO.: 54:8780c-i,8781a-i,8782a-i
TITLE: α-Acylaminoacrylic acids. I. Halogenated derivatives of α-benzamidocrotonic acid and α-benzamidocinnamic acid
AUTHOR(S): Pfleger, Robert; v. Strandtmann, Maximilian
CORPORATE SOURCE: Tech. Hochschule, Bamberg, Germany
SOURCE: Chemische Berichte (1957), 90, 1455-67
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:44595

GI For diagram(s), see printed CA Issue.

AB On halogenation of MeCH:C(NHBz)CO2H (I) and PhCH:C(NHBz)CO2H (II), and their azlactones and esters, the H atom on the C atom of the double bond was replaced by halogen. The halogenated derivs. were converted into compds. of the oxazole and indone series. BzNHCH2CO2H (100 g.) ground with 35 g. fused NaOAc, treated with 200 cc. distilled Ac2O, about 100 cc.
AcH (from 125 cc. paraldehyde and 1 cc. concentrated H2SO4) distilled into the
mixture under ice cooling, the mixture refluxed 2 hrs. at 55-60° (excluding moisture), allowed to stand 12 hrs., another 100 cc. AcH distilled
into the mixture, the whole heated 2.5 hrs. at 55-60° cooled, poured into 2 l. H2O with stirring, and the precipitate washed with a large amount H2O
gave 92 g. O.CPh:N.C(:CXR).CO (III) (R = Me, X = H) (IV), m. 93-6° (MeOH). I (Carter, et al., C.A. 33, 81874) in 8 cc. 2N NaOH treated at 40° with 5.2 cc. Me2SO in 3-4 portions, the mixture shaken vigorously 20 min., allowed to stand overnight, the precipitate filtered off, treated with
aqueous Na2CO3, washed with H2O, dried, and crystallized from a large volume petr.
ether gave 2.5 g. I Me ester, m. 80°. (a) Cl introduced slowly (30 min.) into 10 g. IV in 100 cc. CHCl3 {in the halogenation of III (X = H) the CHCl3 should be free from EtOH, but should however be moist} containing 3
g. precipitated CaCO3 under ice cooling, filtered, the filtrate evaporated in vacuo
below 25°, the residue heated a short time with 7 cc. Ac2O, cooled, and the precipitate recrystd. from Ac2O or C6H6-petr. ether gave 2.48 g. III (R =
Me, X = Cl) (V) m. 127°. (b) RCX:C(NHBz)CO2H (VI) (R = Me, X = Cl) (VII) (1 g.) and 3 cc. Ac2O heated on a boiling H2O bath until a solution formed and cooled gave 750 mg. V. VII treated with concentrated H2SO4, POCl3,
or acyl chlorides gave approx. 80% V. Chlorination of III (R = Ph, X = H)
(VIII) at room temperature by a gave 38% III (R = Ph, X = Cl)(IX), m. 176°. Method b with VI (R = Ph, X = Cl) (X) gave 87% IX. IV in 40 cc. CHCl3 containing 3 g. CaCO3 treated with 2 cc. Br in 10 cc. CHCl3 at the
rate of its decolorization under stirring and worked up as in a gave 2.48 g. III (R = Me, X = Br) (XI), m. 154°. Method b with VI (R = Me, X = Br), gave 90% XI. VIII (5 g.) dissolved in 50 cc. CHCl3, 3 g. CaCO3 added, the mixture treated dropwise at 50-60° during 45 min. in a quartz vessel with simultaneous ultraviolet irradiation with 3 g. Br in

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cc. CHCl3 with stirring and worked up by a gave 2.4 g. III (R = Ph, X = Br) (XII), m. 172°. Method b with VI (R = Ph, X = Br) (XIII) gave 90% XII. A moderate stream of Cl (3 bubbles/sec., tubing 4 mm. diam.) introduced 20 min. into an ice cold soln. of 6 g. IV in 50 cc. CHCl3 contg. 2 g. CaCO3, filtered, the filtrate evapd. in vacuo below 25° the oily residue covered with petr. ether, rubbed, the solid rapidly filtered off, and recrystd. from petr. ether (b. 40-60°) gave 4.2 g. O.CPh:N.CCl(CHClMe).CO, prisms, m. 72-6° (decompn.), deliquescing slowly in the air. (a-1) Finely powd. V (0.5 g.) and 10 cc. satd. (cold) aq. NaHCO3 and some solid NaHCO3 allowed to stand 48 hrs., filtered, the filtrate acidified, and the ppt. recrystd. from AcOH gave 130 mg. VII, m. 186° (decompn.). (b-1) Cl introduced slowly during 25 min. into 200 cc. ice cold AcOH contg. 10 g. I, the AcOH evapd. in vacuo, the residue taken up in aq. NaHCO3, the soln. acidified, and the ppt. recrystd. from 70% AcOH gave 1.38 g. VII. (c-1) IV chlorinated as in
a, the distn. residue treated with 150 cc. H2O, brought into soln. by vigorous stirring and heating slowly in a H2O bath, the soln. filtered hot, and the filtrate allowed to cool slowly gave 2.3 g. VII. (a-2) IX (2
g.) dissolved in 50 cc. 2N NaOH by gentle warming on a H2O bath, acidified
with 2N HCl, the ppt. taken up in aq. NaHCO3, repptd. with HCl, and recrystd. from MeOH gave 0.55 g. VI (R = Ph, X = Cl) (XIV), m. 170° (decompn.). II by b-1 gave 14% XIV. (a-3) XI by a-1 gave 43% VI (R = Me,
X = Br) (XV), m. 174° (decompn.). (b-3) I (2.5 g.) in 50 cc. AcOH treated dropwise with 0.8 cc. Br in 10 cc. AcOH, the AcOH evapd. in vacuo,
the residue taken up in aq. NaHCO3, the soln. acidified and the ppt. crystd. from AcOH gave 350 mg. XV. (c-3) Br (2 cc.) in 10 cc. CHCl3 added
dropwise with stirring to 7 g. XI in 40 cc. CHCl3 at 40° at the rate of its decolorization, the CHCl3 removed in vacuo, the residue mixed with 140 cc. H2O and enough solid NaHCO3 so that the mixt. remained alk. after 24 hrs., the mixt. filtered, the filtrate acidified, and the ppt. recrystd. from AcOH gave 3.8 g. XV. XII by a-2 gave 40% XIII, m. 186° (decompn.). II by b-3 gave 20% XIII. VIII by b-3 at 40-60° with ultraviolet irradiation gave 59% XIII. XII (2.5 g.) in 100 cc. AcOH and 10 cc. concd. HCl boiled 5 hrs., the filtered soln. evapd. in vacuo, the residue extd. with Et2O, and the Et2O-insol. material
recrystd. from H2O gave BzNH2, m. 126-8°. The Et2O ext. extd. with aq. NaHCO3, evapd., and the residue recrystd. from H2O gave BzCH2OH, m. 86°. The NaHCO3 ext. acidified and the product isolated with Et2O gave PhCH2CO2H, m. 78°. Finely powd. V (100 mg.) dissolved in 10 cc. 0.25N MeOH-NaOH at room temp., the soln. treated with 30 cc. H2O, the ppt. filtered off, washed alkali-free, dissolved in hot MeOH, and the soln. treated with H2O to the beginning of turbidity gave 70 mg. VII Me ester (XVI), m. 140°. Cl slowly introduced during 25 min. into 50 cc. ice-cold CHCl3 contg. 5 g. I Me ester (XVII), the soln. evapd. in vacuo, and the residue recrystd. from 80-90% MeOH gave 2.95 g. XVI. XI (1.7 g.) in 250 cc. MeOH heated to boiling, made weakly alk. with 0.1N MeOH-NaOH, after 1 min. the soln. treated with 500 cc. warm H2O, and the product recrystd. from aq. MeOH gave 1.3 g. XV Me ester (XVIII), m. 151°. Br (0.45 cc.) in 10 cc. CHCl3 added dropwise to 25 cc. ice cold CHCl3 contg. 2 g. XVII with stirring, the soln. evapd. in vacuo, and the residue recrystd. from 80% EtOH gave 1.45 g. XVIII. V (100 mg.) dissolved in 10 cc. 0.1N alc. NaOH at 0°, treated with 50 cc. H2O,

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and the ppt. recrystd. from aq. EtOH gave 63 mg. VII Et ester, m. 94°. XI (2 g.) in 40 cc. EtOH heated to boiling, made weakly alk. with 0.1N alc. NaOH, after 1 min. the soln. treated with 100 cc. H2O, and the ppt. recrystd. from aq. EtOH gave 1.5 g. XV Et ester, m. 115°. IX (2.9 g.) in MeOH boiled 2-3 min. and worked up similarly gave 2.75 g. X
Me ester (XIX), m. 167°. A moderate stream of Cl introduced during 2 hrs. into 100 cc. CHCl3 contg. 10 g. II Me ester (XX) at room temp. gave
7.5 g. XIX. XII (6.6 g.) in MeOH treated similarly gave 6.5 g. XIII Me ester (XXI), m. 141°. XX (20 g.) in 150 cc. CHCl3 treated dropwise at room temp. with 4.5 cc. Br in 50 cc. CHCl3 with stirring gave 18 g. XXI. IX (2.8 g.) treated with EtOH and worked up as above gave 2.7 g. X Et ester (XXII), m. 110°. II Et ester (XXIII) (10 g.) in 100 cc. CHCl3 treated 2 hrs. at room temp. with a moderate stream of Cl gave 6.8 g. XXII. XII (6.6 g.) treated with EtOH as above gave 6.2 g. XIII Et ester (XXIV), m. 112°. XXIII (20 g.) in 150 cc. CHCl3 treated with 4.55 cc. Br in 50 cc. CHCl3 at room temp. gave 16 g. XXIV. XVI or XVIII (600 mg.) and 900 mg. anhyd. NaOAc ground together, heated 2.5 hrs. at 160-5° with 10 cc. AcOH in a sealed tube, the mixt. digested several times with 200 cc. Et2O (total amt.), the Et2O-AcOH ext. filtered,
the filtrate evapd. in vacuo, and the residue crystd. from aq. EtOH and then petr. ether gave 120 mg. (from XVI) or 230 mg. (from XVIII) O.CPh:N.C(CO2R'):CR (XXV) (R' = R = Me) (XXVI), m. 94°. XXII or XXIV (4 g.), 4 g. anhyd. NaOAc, and 30 cc. glacial AcOH treated as above (heated 3 hrs. at 160°) gave 1.15 g. (from XXII) or 1.95 g. (from XXIV) XXV (R = Et, R = Ph) (XXVII), m. 101°. When reaction was carried out at 190° and the mixt. steam distd., O.CPh:N.CH:CPh (XXVIII) sepd. out in the condenser while a slight amt. O.CMe:N.CH:CPh was
found in the receiver. XXII or XXIV (2 g.), 3 g. AgF, and 6 g. silica gel
intimately mixed, heated 1 hr. at 140°, extd. with Et2O, the ext. evapd in vacuo, and the residue recrystd. from aq. MeOH gave 0.85 g. (from
XXII) or 1.32 g. (from XXIV) XXVII. XXVI (500 mg.) and 80 cc. N NaOH refluxed 25 min., the soln. filtered hot, the filtrate acidified with HCl,
the resulting emulsion allowed to stand, and the ppt. recrystd. from a large vol. petr. ether gave 400 mg. XXV (R' = H, R = Me).(XXIX), m. 180-1°. XXIX (1 g.), 2 g. silica gel, and 1 g. MgO heated 2 hrs. at 200° in a sealed tube and steam distd. gave 370 mg. O.CPh:N.CH:CMe. XXVII (2 g.) hydrolyzed as above gave 1.1 g. XXV (R' = H,
R = Ph), m. 190° (C6H6), decarboxylation as above yielding 45% XXVIII. VIII (5 g.) brominated as described above but without CaCO3, the ppt. filtered off, and washed with dry CHCl3 gave 2 g. VIII.HBr, m. 150-3° (decompn.); the product must be kept CHCl3-moist and stored under CHCl3; it dissolved in MeOH, EtOH, or AcOH decompg. into HBr and VIII.HBr introduced into dry CHCl3 contg. VIII gave 65% VIII.HBr. III (X = H, R = 3,4-methylenedioxyphenyl) (XXX) (5 g.) in 150 cc. dry CHCl3 treated at 35° during 1 hr. with 2.2 cc. Br in 20 cc. dry CHCl3 under ultraviolet irradiation and after 4-5 hrs. the ppt. filtered off and

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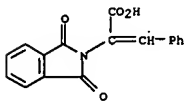


L4 ANSWER 228 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
washed with dry CHCl3 gave 2.2 g. XXX.HBr, m. 175-85° (decompn.). HBr introduced into CHCl3 contg. XXX gave 70% XXX.HBr. The mother liquor from the above bromination of XXX evapd. in vacuo and the residue recrystd. from 5 cc. Ac2O and then C6H6 gave 1.3 g. III (X = Br, R = 3,4-methylenedioxyphenyl), m. 216°. Cl slowly introduced during 50 min. into 300 cc. CHCl3 contg. 10 g. XXX at 40°, the soln. evapd. in vacuo, and the residue crystd. from C6H6 gave 6.3 g. III (X = Cl, R = 3,4-methylenedioxyphenyl), m. 221°. Na phthalimidoacetate (XXXI) (5.8 g.) added portionwise to 5.2 g. phthalimidoacetyl chloride at 100° with stirring, the mixt. kept 15 min. at 100°, cooled, pulverized, heated 0.5 hr6 0°, cooled, added to H2O, the ppt. filtered off, washed with H2O, and pressed on clay plate gave 6.7 g. phthalimidoacetic anhydride (XXXII). XXXII (4.15 g.), 2 g. XXXI, and 5 cc. BzH refluxed 8 hrs. at 180°, distd. in vacuo, the residue steam distd., the residual H2O-insol. material heated 30 min. at 40-50° with 50 cc. 2N NaOH, the soln. filtered, the filtrate acidified, and the product fractionally recrystd. from H2O and then aq. MeOH gave 0.51 g. α-phthalimidocinnamic acid, m. 250° (decompn.). XX (6 g.), 100 cc. abs. MeOH, 3 g. calcined NaZCO3, and 3 cc.
MeI refluxed 20 hrs. excluding moisture (after 10 hrs. an addnl. 3 cc. MeI
added), the mixt. filtered, the filtrate evapd. in vacuo, the residue dissolved in 70 cc. EtOH, the soln. treated with C, filtered, the filtrate
allowed to conc. during 14 days, the resulting cryst. mixt. of large prisms and fine needles sepd. manually, and the former recrystd. from MeOH
gave 2.1 g. N-Me deriv. (XXXIII) of XX, m. 109°. XXIV (5 g.) treated similarly and the product crystd. from a small amt. aq. EtOH gave 3.75 g. N-Me deriv. (XXXIV) of XXIV, m. 98°. XXXIII (3 g.) in 50 cc. 2N NaOH refluxed 15 min., the soln. cooled, filtered, the filtrate acidified with HCl, and the ppt. recrystd. from 80% AcOH gave 2.5 g. PhCX:C(NMeBz)CO2H (XXXV) (X = H) monohydrate (XXXVI), m. 106-7° (decompn.). XXXIV (1 g.) boiled 40 min. with 75 cc. 2N NaOH gave 0.75 g. XXXV (X = Br) (XXXVII), m. 168° (decompn.). XXXVI (1.5 g.) in 100 cc. CHCl3 dried with Na2SO4, the filtered soln. cooled in ice, treated slowly during 30 min. with Cl, evapd. in vacuo, the residue digested 2-3 hrs. with aq. NaHCO3, the soln. filtered, the filtrate acidified, and the ppt. recrystd. from 80% AcOH gave 120 mg. XXXV (X = Cl) (XXXVIII), m. 149°. XXXVIII (350 mg.) and 6 cc. 2% oleum allowed to stand 30-40 hrs. at room temp. with occasional shaking, the soln. poured on ice, the ppt. filtered off, washed with H2O, digested with aq. NaHCO3, and the insol. material recrystd. from EtOH gave 205 mg. CO.C(NMeBz):CX.C:C.CH.CH:CH (XXXIX) (X = Cl), m. 95°. Similarly, 400 mg. XXXVII gave 250 mg. XXXIX (X = Br), m. 122°.

IT 101439-78-5P, Cinnamic acid, α-phthalimido-
RL: PREP (Preparation)
(preparation of)
RN 101439-78-5 CAPLUS
CN Cinnamic acid, α-phthalimido- (6CI) (CA INDEX NAME)

L4 ANSWER 229 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:23060 CAPLUS
DOCUMENT NUMBER: 54:23060
ORIGINAL REFERENCE NO.: 54:4551e-i,4552a-g
TITLE: Tetrazoles. II. The azidolysis of the 5-oxazolones
AUTHOR(S): Behringer, Hans; Grimme, Wolfram
CORPORATE SOURCE: Univ. Munich, Germany
SOURCE: Chemische Berichte (1959), 92, 2967-76
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:23060

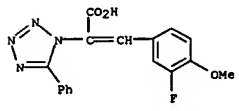
AB cf. C.A. 51, 8079b. The ring cleavage of saturated and unsatd. azlactones
with HN3 yielded α-(1-tetrazolyl)propionic acid and α-(1-tetrazolyl)acrylic acids, resp. 2-Methyl-4-benzal-5-oxazolone (I) (18.7 g.) and 29 g. NaN2 in 250 cc. dry tetrahydrofuran treated slowly
with 20 g. AlCl3 in 250 cc. tetrahydrofuran, stirred 10 hrs. on the water bath, cooled, treated with stirring with 125 cc. 6N HCl in portions, stirred 1 hr., the organic layer worked up, the residue kept overnight, dissolved in aqueous NaHCO3, boiled with C, filtered, and acidified with HCl
gave 7-9 g. α-(5-methyl-1-tetrazolyl)cinnamic acid (II), m. 198° (decomposition) (1:10 HCONMe2-H2O). I (6.22 g.) added to 43 cc. 1.13M HN3 in CHCl3, kept 10 hrs. at room temperature, and filtered yielded 7.2
g. II. p-MeO derivative (2.95 g.) of I gave similarly 2.8 g. 4-MeO derivative of
II, needles, m. 186° (decomposition) (20% aqueous EtOH). p-Cl derivative (0.6
g.) of I gave 0.50 g. 4-Cl derivative of II, leaflets, m. 189° (decomposition) (20% aqueous EtOH). 4-Isobutylidene derivative (4.0 g.) of I gave 4.6
g. α-(5-methyl-1-tetrazolyl)-γ,γ-dimethylcrotonic acid, needles, m. 164° (decomposition) (H2O). 4-Benzal-2-phenyl-5-oxazolone (III) (5.0 g.) gave similarly during 5 days at room temperature 4.13 g. α-(5-phenyl-1-tetrazolyl)cinnamic acid (IV) and 0.91 g. unchanged III. A similar run in a sealed tube at 110-15° during 5 hrs. gave 3.44 g. IV, m. 191-2° (decomposition) (iso-PrOH), and 1.39 g. N-containing,
neutral product, m. 184.5-85° (MeOH), which was not investigated further. 4-(p-Methoxybenzal)-2-phenyl-5-oxazolone (V) (3.0 g.) added to 0.50 g. HN3 in 15 cc. CHCl3, kept 4 days at room temperature, treated with 1.04
g. HN3 in 20 cc. CHCl3, allowed to stand 3 days, and worked up gave 2.36 g. α-(5-phenyl-1-tetrazolyl)-4-methoxycinnamic acid (VI), m, 181.5-2.5° (decomposition) (iso-PrOH), and 0.71 g. unchanged V. A similar run with 3.0 g. V and 0.50 g. HN3 in 15 cc. CHCl3 gave during 2 hrs. at 115° in a sealed tube 2.33 g. VI and 0.87 g. V. 2-Phenyl-4-(p-chlorobenzal)-5-oxazolone (VII) (1.72 g.) treated 2 days at room temperature with NH3 gave 0.45 g. unchanged VII and 0.77 g. α-(5-phenyl-1-tetrazolyl)-4-chlorocinnamic acid, m. 188° (decomposition) (80% EtOH).
2-Phenyl-4-(3-fluoro-4-methoxybenzal)-5-oxazolone
(VIII) (2.33 g.) and HN3 in CHCl3 heated 5 hrs. at 115° in a sealed tube gave 0.26 g. unchanged VIII and 2.24 g. α-(5-phenyl-1-tetrazolyl)-3-fluoro-4-methoxycinnamic acid, m. 194.5-5.5° (decomposition) (EtOH). Powdered 2-phenyl-4-(m-nitrobenzal)-5-oxazolone (IX)

L4 ANSWER 229 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(5.64 g.) and the calcd. amt. of HN3 in CHCl3 kept 8 days at room temp. with occasional shaking and worked up in the usual manner yielded 3.24 g. unchanged IX and 2.05 g. α-(5-phenyl-1-tetrazolyl)-3-nitrocinnamic acid (X), m. 163-4° (decompn.) (abs. EtOH). A similar run in a sealed tube at 115° during 5 hrs. yielded 5.09 g. X. p-Isomer (XI) of IX (5.64 g.) in 20 cc. CHCl3 treated with 15 cc. HN3-CHCl3 (contg. 76 g. HN3/l.), kept 8 days at room temp. in a sealed tube, shaken 1 week during the day, and worked up in the usual manner gave 4.1 g. unchanged XI, m. 239.5-40.5° (xylene), and 1.36 g. crude acid; the crude acid extd. with satd. aq. NaHCO3 and the ext. acidified gave 0.22 g. p-O2NC6H4CH:C(NHBz)CO2H (XII), needles, m. 250-2° (dioxane); the undissolved portion washed with H2O and the washings acidified gave 0.67 g. mixt. of XII and 0.48 g. light-sensitive α-(5-phenyl-1-tetrazolyl)-4-nitrocinnamic acid (XIII), yellowish, m. 200-2° (decompn.) with browning and sintering (MeOH). XI (5.64 g.) in 30 cc. CHCl3 treated with 15 cc. CHCl3 contg. 76 g. HN3/l., heated 10.5 hrs. in a
sealed tube at 110-15°, cooled, and worked up in the usual manner with aq. NaHCO3 gave 0.46 g. unchanged XI and 1.52 g. pure XIII. 2-(p-Nit
rophenyl)-4-benzal-5-oxazolone (XIV) (4.23 g.) and 0.76 g. HN3 in 10 cc. CHCl3 shaken 1 hr. in a sealed tube, kept 1 month at room temp., and worked up with aq. NaHCO3 gave 3.70 g. unchanged XIV, m. 234-5° (dioxane), and 0.43 g. α-[5-(p-nitrophenyl)-1-tetrazolyl]cinnamic acid (XV), m. 247-8° (decompn.) (dioxane). XIV (5.64 g.) and 1.0 g. HN3 in 16 cc. CHCl3 heated 5 hrs. at 110° in a sealed tube, cooled, filtered from 2.35-2.40 g. unchanged XIV, evapd., dissolved in Et2O, and worked up with aq. NaHCO3 gave 1.40-1.55 g. neutral, viscous, brown resin, and 0.63-0.69 g. acid, m. 218-20° (abs. EtOH). NaOH (0.7 g.), 1.1 cc. 30% H2O2, and 1 g. II in 50 cc. H2O kept 5 hrs. at room temp. and acidified with 2N HCl gave 3-phenyl-2-(5-methyl-1-tetrazolyl)-2-
carboxyoxirane (XVI), m. 153° (decompn.). XVI (1.0 g.) in 25 cc. 2N H2SO4 warmed 1 hr., cooled, treated with 200 cc. 0.182N HIO4, dild. to 250 cc., kept overnight, a 230-cc. portion steam distd., and the distillate treated with 2,4-(O2N)2C6H3NH-NH2 in EtOH-H2SO4 (yielded 386 mg. 2,4-(O2N)2C6H6NHN:CHPh, m. 238-9° (EtOH); the distn. residue adjusted with NaOAc to pH 3, treated at 50° with excess aq. CuSO4, kept overnight, filtered, the residue washed with H2O, suspended in boiling H2O, treated with H2S, filtered, concd. on the steam bath, evapd.,
and the residue sublimed at 95°/0.001 mm. gave 5-methyltetrazole, m. 145°. 2-Methyl-4-benzyl-5-oxazolone (6.0 g.) and 19 cc. 2M HN3-CHCl3 kept 10 hrs. at room temp., evapd., and the glassy residue worked up with aq. NaHCO3 gave 2.8 g. α-(5-methyl-1-tetrazolyl)-β-phenylpropionic acid (XVII), leaflets, decomp. 178° (H2O). II (401 mg.) in 12 cc. 85% MeOH hydrogenated at room temp. over 10 mg. PtO2 gave 391 mg. XVII, decomp. 176°. 2-Methyl-4-isobutyl-5-oxazolone (5.3 g.) and 21 cc. 2M HN3-CHCl3 kept 10 hrs. at room temp. and worked up in the usual manner gave 2.2 g. α-(5-methyl-1-tetrazolyl)-γ,γ-dimethylbutyric acid, needles, m. 127° (decompn.) (H2O).

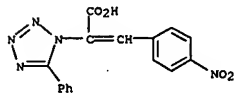
IT 1547-79-1P, 1H-Tetrazole-1-acetic acid, α-(3-fluoro-4-methoxybenzylidene)-5-phenyl- 1738-45-0P, 1H-Tetrazole-1-acetic acid, α-p-nitrobenzylidene-5-phenyl- 1738-46-1P,

L4 ANSWER 229 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
1H-Tetrazole-1-acetic acid, α-m-nitrobenzylidene-5-phenyl- 1738-48-3P, 1H-Tetrazole-1-acetic acid, α-p-methoxybenzylidene-5-phenyl- 1738-50-7P, 1H-Tetrazole-1-acetic acid, α-benzylidene-5-methyl- 1738-51-8P, 1H-Tetrazole-1-acetic acid, α-p-chlorobenzylidene-5-methyl- 1738-53-0P, 1H-Tetrazole-1-acetic acid, α-p-methoxybenzylidene-5-methyl- 1738-65-4P, 1H-Tetrazole-1-acetic acid, α-benzylidene-5-phenyl- 1738-66-5P, 1H-Tetrazole-1-acetic acid, α-p-chlorobenzylidene-5-phenyl- 101727-98-4P, 1H-Tetrazole-1-acetic acid, α-benzylidene-5-(p-nitrophenyl)-
RL: PREP (Preparation)
(prepn. of)

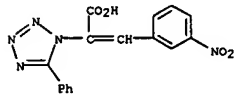
RN 1547-79-1 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(3-fluoro-4-methoxybenzylidene)-5-phenyl- (6CI, 8CI) (CA INDEX NAME)



RN 1738-45-0 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-[(4-nitrophenyl)methylene]-5-phenyl- (9CI) (CA INDEX NAME)

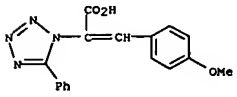


RN 1738-46-1 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(m-nitrobenzylidene)-5-phenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

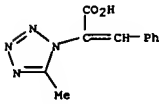


L4 ANSWER 229 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

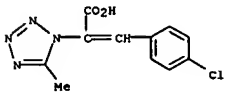
RN 1738-48-3 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-methoxybenzylidene)-5-phenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)



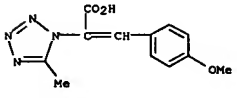
RN 1738-50-7 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-methyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)



RN 1738-51-8 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-chlorobenzylidene)-5-methyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

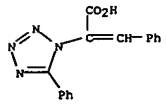


RN 1738-53-0 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-methoxybenzylidene)-5-methyl- (6CI, 7CI, 8CI) (CA INDEX NAME)

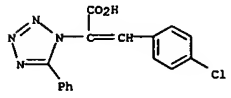


RN 1738-65-4 CAPLUS
CN 1H-Tetrazole-1-acetic acid, 5-phenyl-α-(phenylmethylene)- (9CI) (CA INDEX NAME)

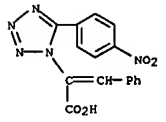
L4 ANSWER 229 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 1738-66-5 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-(p-chlorobenzylidene)-5-phenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)



RN 101727-98-4 CAPLUS
CN 1H-Tetrazole-1-acetic acid, α-benzylidene-5-(p-nitrophenyl)- (6CI) (CA INDEX NAME)



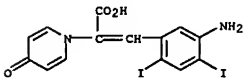
L4 ANSWER 230 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:2241 CAPLUS
DOCUMENT NUMBER: 54:2241
ORIGINAL REFERENCE NO.: 54:530d-i,531a-c
TITLE: Isonicotinoylacetic ester and its derivatives. II. Condensation with aldehydes and amines
AUTHOR(S): Magidson, O. Yu.
CORPORATE SOURCE: S. Ordzhonikidze All-Union Chem. Pharm. Sci. Research Inst., Moscow
SOURCE: Zhurnal Obshchei Khimii (1959), 29, 165-74
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:2241

AB cf. C.A. 50, 16764c. To 9.7 g. Et isonicotinoylacetate in 20 ml. EtOH there was added at 10° 2 ml. formalin and after 3 hrs. the mixture was heated 4 hrs. on a steam bath, concentrated in vacuo and heated 3 hrs. with 10 ml. 6N HCl; after neutralization with 30% NaOH, there separated 78% 1,3-diisonicotinoylpropane (I), m. 92-3°; mono-HCl salt, decomposing 254-6°; di-HCl salt is very soluble; dioxime, m. 197-8° (80% EtOH). Heating 3 g. I with 2 g. HONH2.HCl and 10 ml. 90% EtOH in a sealed tube 7 hrs. at 160° gave 38% 2,6-bis(4-pyridyl)pyridine, HCl salt tetrahydrate, m. 280-5°; free base, m. 144-6° (EtOAc). The infrared spectrum of the substance is shown. The free base also forms a very soluble di-HCl salt and a picrate, decomposing 252-4°. Reduction of I with (iso-PrO)3Al-iso-PrOH 4 hrs. on a steam bath gave after the usual treatment 82% glassy 1,5-di(4-pyridyl)pentanediol, b0.5 242-5°. Heating 7.7 g. Et isonicotinoylacetate with 3 g. m-O2NC6H4CHO in 5 ml. EtOH 4 hrs. with slow distillation of the solvent gave, after an aqueous treatment and refluxing the product 3 hrs. with 5:3 HCl, 1,3-diisonicotinoyl-2-(m-nitrophenyl)propane, m. 151-2° (MeOH); dioxime, m. 258-60°. Heating 9.7 g. Et isonicotinoylacetate with 5.8 g. BzH and 1 drop piperidine 3 hrs. on a steam bath gave after treatment with 5% HCl, followed by 10% NaOH, α,α'-diisonicotinoyl-β-phenylglutaric acid di-Et ester (II), m. 102-3°, and Et benzyli deneisonicotinoylacetate (III), m. 110-12°, separated by crystallization from 70% MeOH. The former refluxed with 20% HCl gave 2-phenyl-1,3-diisonicotinoylpropane, m. 103° (monohydrate), m. 108-10° (anhydrous). An attempt to form the oxime of II gave 3-(4-pyridyl)isoxazolone, decomposing 194-5°, which also formed in a similar attempt made with III. Condensation of Et isonicotinoylacetate (IV) with salicylaldehyde in EtOH gave a little isonicotinoylacetylisonicotinoylacetic acid, m. 261-2°. A mixture of 9.6 g. IV with 8.3 g. CCl3CHO.H2O gave after 3 hrs. on a steam bath with 10 ml. AcOH and after dilution with 10 ml. H2O after cooling, a solid mass which was extracted with EtOAc to give 4-C5H4NCOCH(CHOHCCl3)CO2Et, m. 139-41° (EtOAc); this, heated with 20% HCl gave γ-pyridyl 3,3,3-trichloro-2-hydroxypropyl ketone, m. 177-8°, and a small amount of a substance, m. 307-10°, which was not identified. Heating 9.5 g. I with 3.7 g. p-Me2NC6H4CHO in 5 ml. AcOH 4 hrs. at 120° gave 3.3 g. yellow 2,5-diisonicotinoyl-3-(p-dimethylaminophenyl)glutaric acid

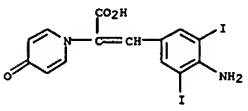
L4 ANSWER 230 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
di-Et ester, m. 137-8°. Heating 8.6 g. o-C6H4(NH2)2 and 15.4 g. I in xylene to 145-50° with gradual distn. of low boiling materials gave 15.5 g. 2-benzimidazolylmethyl γ-pyridyl ketone, m. 211-12°; HCl salt, m. 230-5°. Hydrogenation of 9.5 g. m-nitro-p-anisidine in EtOH over Pt at normal pressure, rapid filtration and treatment of the filtrate with 11.5 g. I, followed by addn. of 40 ml. xylene and heating to 150° with slow distn. gave a solid, which was extd. with MeOH at reflux; the cooled ext. gave a yellow ppt. while the filtrate on acidification with HCl and kept 2 days gave a ppt. which was taken up in hot 5% HCl and treated with AcONa to yield a red ppt.; this treated with NH4OH gave 3 g. yellow 2[4(5)-methoxybenzimidazolyl]methyl 4-pyridyl ketone, m. 317-19° (C5H5N); di-HCl salt, yellow, m. 275-7°. Refluxed with 48% HBr 5 hrs. this gave yellow-green 2-[4(5)-hydroxybenzimidazolyl]methyl 4-pyridyl ketone tri-HBr salt, does not m. 370°; the mother liquor gave more of this product which treated with H2O gave red mono-HBr salt; treated with NaOH this gave a yellow solid of the free base, does not m. 370°.

IT 106652-52-2P, 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- 106652-69-1P, 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 106652-52-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-69-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

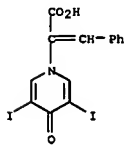


L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:2240 CAPLUS
DOCUMENT NUMBER: 54:2240
ORIGINAL REFERENCE NO.: 54:530a-d
TITLE: Studies on the chemistry of radioopaque compounds. I. α-[N-(4-Pyridonyl)]cinnamic acids and their iodo derivatives
AUTHOR(S): Bojarska-Dahlig, Halina
CORPORATE SOURCE: Inst. Farmaceutyczny, Warsaw
SOURCE: Roczniki Chemii (1959), 33, 589-603
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The following α-[N-(4-pyridonyl)]- (I) and α-[N-(3,5-diiodo-4-pyridonyl)]cinnamic acids (II) were prepared by the reaction of benzaldehyde (III) or substituted III with Na salts of 4-pyridone-N-acetic acid (IV) or 3,5-diiodo derivative of IV in presence of excess of acetic anhydride at 140-50° (modified Perkin synthesis) (compound, m.p., and % yield given): I, 271-2°, 54; I 3-nitro derivative (V), 208-9°, 92; I 3-methoxy derivative, 375.5-8.5°, 55; I 3-hydroxy derivative, 249.5-51°, 66; I 4-nitro derivative (VI), 279.5-80.5°, 73; I 4-methoxy derivative, 276-8°, 53; I 4-hydroxy derivative, 251.5-2.5°, 44; I 2-chloro derivative, 217-18°, 65; II, 278-80°, 77; II 3-nitro derivative (VII), 281.5-2.5°, 95; II 4-nitro derivative (VIII), decomposed, 74; II 4-methoxy derivative, 266-7°, 67; II 2-chloro derivative, 254-5°, 84. All the compds. melted with decomposition V, VI, VII and VIII were reduced to the amino derivs.: 281-2°, 92%; 243-4°, 88%; decomposed, 82%; and 266.5°, 69%. These were iodinated by ICl to give: 4,6(?)-diiodo-3-amino, 243-4.5°, 98; 3,5-diiodo-4-amino derivs. of I, decomposed, 97; 4,6(?)-diiodo-3-amino, 289-91°, 99; 3-iodo-4-amino derivs. of II, decomposed, 96. The iodo derivs. were tested on dogs for cholecystographic properties. The results were neg. on administration per os, but pos. on intravenous administration of aqueous solns. of their N-methylglucamine salts.

IT 100873-29-8, 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo-
(and derivs.)

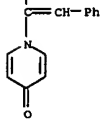
RN 100873-29-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



IT 100725-76-6, 1(4H)-Pyridineacetic acid, α-benzylidene-4-oxo-

L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(and iodine-contg. derivs.)

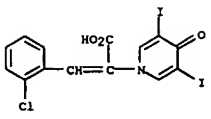
RN 100725-76-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-benzylidene-4-oxo- (6CI) (CA INDEX NAME)



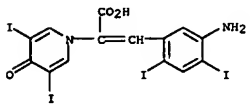
IT 100540-95-2P, 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- 100541-48-8P, 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- 100873-32-3P, 1(4H)-Pyridineacetic acid, α-(4-amino-3-iodobenzylidene)-3,5-diiodo-4-oxo- 100961-30-6P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- 101094-71-7P, 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-4-oxo- 101278-67-5P, 1(4H)-Pyridineacetic acid, α-(5-acetamido-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- 106590-29-8P, 1(4H)-Pyridineacetic acid, α-p-nitrobenzylidene-4-oxo- 106590-61-8P, 1(4H)-Pyridineacetic acid, α-m-nitrobenzylidene-4-oxo- 106652-51-1P, 1(4H)-Pyridineacetic acid, α-[p-aminobenzylidene]-3,5-diiodo-4-oxo- 106652-52-2P, 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- 106652-68-0P, 1(4H)-Pyridineacetic acid, α-[m-aminobenzylidene]-3,5-diiodo-4-oxo- 106652-69-1P, 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo- 106782-71-2P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-nitrobenzylidene-4-oxo- 106783-04-4P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-m-nitrobenzylidene-4-oxo- 107558-27-0P, 1(4H)-Pyridineacetic acid, α-p-hydroxybenzylidene-4-oxo- 107558-89-4P, 1(4H)-Pyridineacetic acid, α-m-hydroxybenzylidene-4-oxo- 107920-25-2P, 1(4H)-Pyridineacetic acid, α-[p-aminobenzylidene]-4-oxo- 107922-11-2P, 1(4H)-Pyridineacetic acid, α-[m-aminobenzylidene]-4-oxo- 108620-58-2P, 1(4H)-Pyridineacetic acid, α-p-methoxybenzylidene-4-oxo- 108621-67-6P, 1(4H)-Pyridineacetic acid, α-m-methoxybenzylidene-4-oxo- 860411-11-6P, 1(4H)-Pyridineacetic acid, α-(m-acetamidobenzylidene)-3,5-diiodo-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 100540-95-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

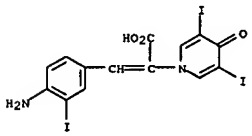
L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



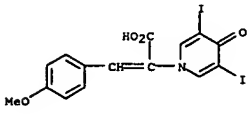
RN 100541-48-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



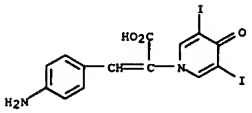
RN 100873-32-3 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-amino-3-iodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



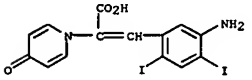
RN 100961-30-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- (6CI) (CA INDEX NAME)



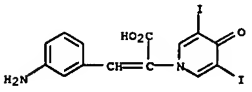
L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



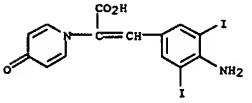
RN 106652-52-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-amino-2,4-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-68-0 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-aminobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



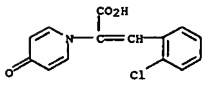
RN 106652-69-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-amino-3,5-diiodobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



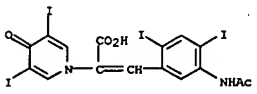
RN 106782-71-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(p-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

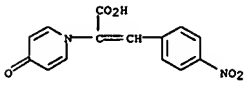
RN 101094-71-7 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-4-oxo- (6CI) (CA INDEX NAME)



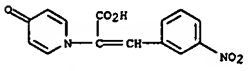
RN 101278-67-5 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(5-acetamido-2,4-diiodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



RN 106590-29-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

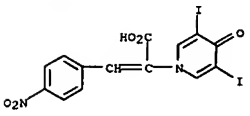


RN 106590-61-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

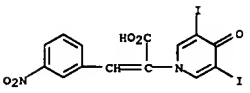


RN 106652-51-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-aminobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

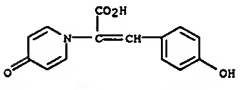
L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



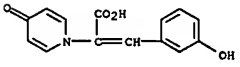
RN 106783-04-4 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(m-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



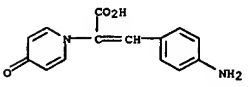
RN 107558-27-0 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-hydroxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



RN 107558-89-4 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-hydroxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

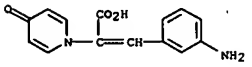


RN 107920-25-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-aminobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)

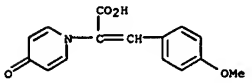


L4 ANSWER 231 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

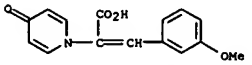
RN 107922-11-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-aminobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



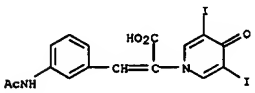
RN 108620-58-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-methoxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



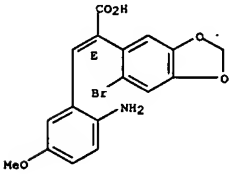
RN 108621-67-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-methoxybenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



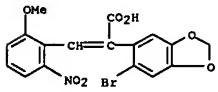
RN 860411-11-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-acetamidobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



L4 ANSWER 232 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 232 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:1971 CAPLUS
DOCUMENT NUMBER: 54:1971
ORIGINAL REFERENCE NO.: 54:401f-h
TITLE: 2-Nitro-6-methoxybenzaldehyde
AUTHOR(S): Pettit, Geo. R.
CORPORATE SOURCE: Univ. of Maine, Orono
SOURCE: Journal of Organic Chemistry (1959), 24, 866-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The synthesis of trans-2-amino-6-methoxy-α-(3,4-methylenedioxy-6-bromophenyl)cinnamic acid (I) from 2-nitro-6-methoxybenzaldehyde (II) was described. 2-Methyl-3-nitrophenol (73 g.) in 400 ml. H2O containing 19 g. NaOH was treated with 60 g. Me2SO4, heated 2 hrs. on the steam bath, and the crude mixture steam distilled to give 42 g. 2-nitro-6-methoxytoluene (III), m. 55-7.5°. III (40 g.) in 250 ml. CS2 added during 0.5 hr. to 70 g. chromyl chloride in 150 ml. CS2, left 72 hrs. at room temperature, the solid immediately collected, washed, the solid added to H2O, and extracted with CHCl3 gave 15 g. II, m. 110-11° (CCl4), λ 5.85 μ. II (2 g.), 3.06 g. 6-bromohomopiperonylic acid, 10 ml. Ac2O, and 1 ml. NEt3 was refluxed 15 min. to give 0.87 g. 2-nitro analog (IV) of I, yellow crystals, m. 264-5° (decomposition), λ 5.95 μ. IV (0.55 g.) in 3.3 g. FeSO4, 0.2 ml. HCl, and 5 ml. H2O heated to 90-5° before addition of 3 ml. 28% NH4OH, the mixture heated a further 45 min., filtered hot, and the filtrate acidified gave 0.41 g. I, m. 205-6° (MeOH-H2O), λ 5.95 μ.
IT 130862-09-8P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)- 876659-16-4P, Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans-
RL: PREP (Preparation)
(preparation of)
RN 130862-09-8 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)- (6CI) (CA INDEX NAME)



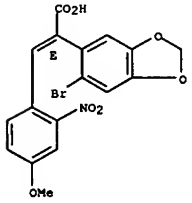
RN 876659-16-4 CAPLUS
CN Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:72502 CAPLUS
DOCUMENT NUMBER: 53:72502
ORIGINAL REFERENCE NO.: 53:13124a-g
TITLE: Phenanthrene derivatives. II. Synthesis of 3-methoxy-5,6(and 6,7)-methylenedioxyphenanthrene
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi
CORPORATE SOURCE: Nagoya City Univ.
SOURCE: Yakugaku Zasshi (1959), 79, 245-8
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Na homopiperonylate (I) (5.8 g.), 5.2 g. 2,4-O2N(MeO)C6H3CHO (II), and 25 ml. Ac2O heated 20 hrs. at 120°, heated 30 min. with 50 ml. H2O, the AcOH removed in vacuo, the residue taken up in 500 ml. 5% NH4OH, washed with Et2O, and the solution acidified with HCl yielded 6.8 g. trans-α-(3,4-methylenedioxyphenyl)-2-nitro-4-methoxycinnamic acid (III), columns, m. 212-13° (EtOH), and the mother liquor gave 0.5 g. cis-isomer (IV) of III, m. 237°. FeSO4.7H2O (4.4 g.) in 10 ml. H2O and 12 ml. concentrated NH4OH treated dropwise with 1 g. III in 20 ml. 5% NH4OH, heated 10 min. on a H2O bath, the solution filtered, and the filtrate treated with HCl to pH 5 gave 0.8 g. 2-NH2 analog (V) of III, granules, m. 202-3° (decomposition) (EtOH). Similarly, 0.5 g. IV yielded 0.3 g. 3-(3,4-methylenedioxyphenyl)-7-methoxycarbostyril (VI), needles, m. 272°. Or, 0.8 g. V in 50 ml. pure EtOH refluxed 2 hrs., and the solution concentrated gave 0.6 g. VI, m. 272° (EtOH). V (1 g.) in 40 ml. MeOH and 12.5 ml. 20% H2SO4 at 0° diazotized with 10 ml. N NaNO2, kept 30 min., 15 ml. H2O added, 3 g. Cu added portionwise, stirred until the evolution of N ceased, heated 30 min. on a H2O bath, the solution made alkaline with NH4OH, concentrated, and the product extracted with Et2O gave 0.3 g. 3-methoxy-6,7-methylenedioxy-9-phenanthrenecarboxylic acid (VII), needles, m. 324-5° (decomposition) (EtOH); the mother liquor concentrated gave 0.05 g. 5,6-CH2O2 analog (VIII) of VII, needles, m. 266-8° (decomposition). 6,3,4-Br(CH2O2)C6H2CH2CO2Na (2.8 g.), 1.8 g. II, and 20 ml. Ac2O treated as in III gave 2.8 g. trans-α-(2-bromo-4,5-methylenedioxyphenyl)-2-nitro-4-methoxycinnamic acid (IX), granules, m. 204°. FeSO4.7H2O (13.2 g.) in 30 ml. H2O and 36 ml. concentrated NH4OH treated with 2 g. IX in 40 ml. 5% NH4OH and the product treated as in V yielded 1.3 g. 2-NH2 analog (X) of IX, granules, m. 207-8° (decomposition). X (1.3 g.) in 24 ml. MeOH and 15 ml. 20% H2SO4 diazotized with 12 ml. N NaNO2 gave 0.4 g. 1-bromo-3,4-methylenedioxy-6-methoxy-10-phenanthrenecarboxylic acid (XI). X (1 g.) in 20 ml. EtOH refluxed 10 hrs. and cooled gave 0.5 g. 3-(2-bromo-4,5-methylenedioxyphenyl)-7-methoxycarbostyril (XII), needles, m. 284-5°. Catalytic reduction of 0.4 g. IX in 40 ml. EtOH and 40 ml. 10% KOH-EtOH with 0.3 g. Pd-C yielded 0.2 g. VIII, m. 266-8° (decomposition). VIII (0.2 g.) in 10 ml. C9H7N and 0.2 g. Cu heated 10 min. at 180-200° and 20 min. at 250-60°, cooled, Et2O added, washed with dilute HCl, neutralized with 5% NaOH, the Et2O removed, and the residue in C6H6 passed through Al2O3 gave 0.06 g. 3-methoxy-5,6-methylenedioxyphenanthrene (XIII), needles, m. 134° (EtOH);

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
picrate, needles, m. 172-3° (decompn.). Similarly 0.1 g. VII as above yielded 0.02 g. 6,7-CH2O2 analog of XIII, needles, m. 135-6°; picrate m. 161-2° (decompn.).
IT 130862-01-0P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(4-methoxy-2-nitrophenyl)-, trans- 876659-18-6P, Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- 876659-46-0P, Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)-, trans- 876659-64-2P, Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- 876659-65-3P, Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, cis-
RL: PREP (Preparation)
(preparation of)
RN 130862-01-0 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(4-methoxy-2-nitrophenyl)-, trans- (6CI) (CA INDEX NAME)

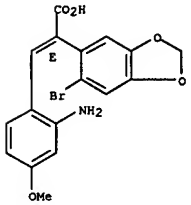
Double bond geometry as shown.



RN 876659-18-6 CAPLUS
CN Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

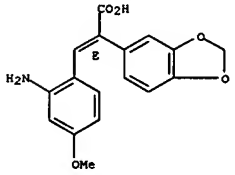
Double bond geometry as shown.

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 876659-46-0 CAPLUS
CN Acrylic acid, 3-(2-amino-4-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

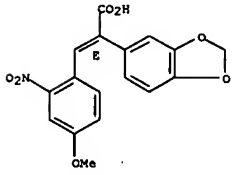
Double bond geometry as shown.



RN 876659-64-2 CAPLUS
CN Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

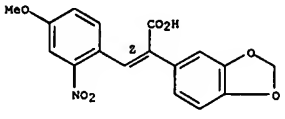
Double bond geometry as shown.

L4 ANSWER 233 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 876659-65-3 CAPLUS
CN Acrylic acid, 3-(4-methoxy-2-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-, cis- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 234 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:72501 CAPLUS
DOCUMENT NUMBER: 53:72501
ORIGINAL REFERENCE NO.: 53:13123d-i,13124a-b
TITLE: Phenanthrene derivatives. I. Synthesis of 3,4-methylenedioxyphenanthrene
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi
CORPORATE SOURCE: Nagoya City Univ.
SOURCE: Yakugaku Zasshi (1959), 79, 241-4
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 3,4-CH2O2C6H3CH2CO2Na (I) (6.7 g.), 5 g. 2-O2NC6H4CHO, and 33 ml. Ac2O heated 20 hrs. at 120°, the product heated 30 min. with 50 ml. H2O, the AcOH removed in vacuo, the residue treated with 500 ml. 5% NH4OH, washed with Et2O, and the solution acidified with HCl gave 4.2 g. trans-2-O2NC6H4CH:C(C6H3O2CH2-3,4)CO2H (II), columns, m. 224-5° (EtOH); the mother liquor concentrated gave 1.4 g. cis analog (III) of II, columns, m. 192-3°. FeSO4.7H2O (4.4 g.) in 10 ml. H2O and 12 ml. concentrated NH4OH treated dropwise with 1 g. II in 20 ml. 5% NH4OH, heated 10 min. on a H2O bath, the solution filtered while hot, and the filtrate treated with concentrated HCl to pH 5 gave 0.8 g. 2-NH2 analog (IV) of II, granules, m. 208° (decomposition) (EtOH). Similarly, 0.5 g. III yielded 0.3 g. 3-(3,4-methylenedioxyphenyl)carbostyril (V), needles, m. 256-7°. Or, 1 g. IV, 10 ml. Ac2O, and 1 ml. concentrated H2SO4 heated 30 min. at 100°, cooled, heated 30 min. with 50 ml. H2O, and the solution neutralized with NaHCO3 yielded 0.7 g. V, needles, m. 256-7° (EtOH). IV (1 g.) in 20 ml. MeOH and 12.5 ml. 20% H2SO4 at 0° diazotized with 10 ml. N NaNO2, kept 30 min., the solution with 15 ml. H2O treated portionwise with 3 g. Cu, stirred until the evolution of N ceased, made alkaline with NH4OH, the solution concentrated, the residue acidified with HCl, and the product extracted with Et2O gave 0.38 g. 2,3-methylenedioxy-10-phenanthrenecarboxylic acid (VI), needles, m. 212-13° (decomposition) (EtOH); the mother liquor concentrated gave 0.02 g. 3,4-CH2O2 analog (VII) of VI, needles, m. 267° (decomposition). VI (0.12 g.) in 10 ml. C9H7N and 0.2 g. Cu heated 10 min. at 180-200° and 20 min. at 250-60°, the solution diluted with Et2O, washed with dilute HCl, neutralized with 5% NaOH, the Et2O removed, and the residue in C6H6 passed through Al2O3 gave 0.06 g. 2,3-methylenedioxyphenanthrene (IX), columns, m. 93-4°; picrate m. 151-2° (EtOH). Similarly, 0.1 g. VII yielded 0.03 g. 3,4-methylenedioxyphenanthrene (X), columns, m. 70-1°; picrate, red brown needles, m. 168° (decomposition). The free acid (18 g.) of I in 200 ml. CHCl3 treated dropwise with 16 g. Br at 10-15°, kept 2 hrs., and the product recrystd. (C6H6) gave 20.2 g. 6,3,4-Br(CH2O2)C6H2CH2CO2H (XI), needles, m. 190°. Na salt (10.4 g.) of XI, 5.6 g. 2-O2NC6H4CHO, and 35 ml. Ac2O treated as in II gave 9.4 g. trans-α-(2-bromo-4,5-methylenedioxyphenyl)-2-nitrocinnamic acid (XII), columns, m. 237°. FeSO4.7H2O (6.6 g.) in 15 ml. H2O and 18 ml. concentrated NH4OH treated dropwise with 1 g. XII in 20 ml. 5% NH4OH and the product treated as in IV yielded 0.7 g. 2-NH2 analog (XIII) of XII,

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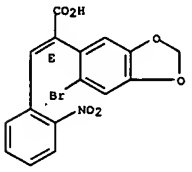
granules, m. 223°. XIII (1 g.) in 10 ml. Ac2O and 1 ml. concd. H2SO4 gave product which treated as for V yielded 0.7 g. 3-(2-bromo-4,5-methylenedioxyphenyl)carbostyril (XIV), granules, m. 279-80°. XIII (2.4 g.) in 48 ml. MeOH and 30 ml. 20% H2SO4 diazotized with 24 ml. N NaNO2 gave 0.8 g. 1-bromo-3,4-methylenedioxy-10-phenanthrenecarboxylic acid (XV). Reducing 0.2 g. XV in 20 ml. EtOH and 20 ml. 10% KOH-EtOH with 0.2 g. Pd-C, concg. the soln., extg. the residue with H2O, acidifying with HCl, and extg. with Et2O gave 0.11 g. VII, needles, m. 267° (decompn.). VII (0.2 g.) in 20 ml. C9H7N treated with 0.3 g. Cu as in X yielded 0.05 g. X, m. 70-1°; picrate m. 168° (decompn.).

IT 131410-39-4P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- 132727-18-5P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, cis- 132727-19-6P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- 876659-42-6P, Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- 876659-44-8P, Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans-
RL: PREP (Preparation)
(preparation of)

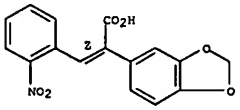
RN 131410-39-4 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 132727-18-5 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, cis- (6CI) (CA INDEX NAME)

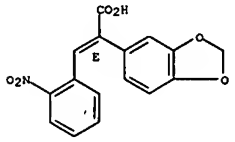
Double bond geometry as shown.



L4 ANSWER 234 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

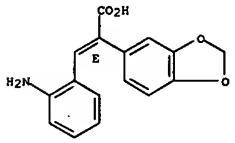
RN 132727-19-6 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



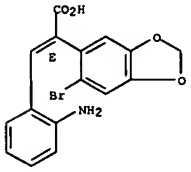
RN 876659-42-6 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 876659-44-8 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-, trans- (6CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 234 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 235 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1959:62535 CAPLUS
DOCUMENT NUMBER: 53:62535
ORIGINAL REFERENCE NO.: 53:11325i,11326a-i,11327a-f
TITLE: Plant substances containing a nitro group. III. The synthesis of a degradation product of aristolochic acid-II, 3,4-methylenedioxy-10-acetamidophenanthrene
AUTHOR(S): Pailer, M.; Schleppnik, A.
SOURCE: Monatshefte fuer Chemie (1958), 89, 175-85
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:62535

AB cf. C.A. 52, 1979e. Aristolochic acid-II, obtained from Aristolochia clematitis, previously (loc. cit.) identified as 3,4-methylenedioxy-10-nitrophenanthrene-1-carboxylic acid, has been degraded by decarboxylation, acetylation, and reduction, to 3,4-methylenedioxy-10-acetamidophenanthrene (I). Piperonylidenerhodanine (II) was obtained in 93% yield when 60 g. piperonal and 51 g. rhodanine in 800 ml. boiling AcOH was treated with 200 g. anhydrous AcONa, stirred 30 min. at boiling, cooled, and poured into 4 l. H2O. The crystals were washed with water and dried at 110° to yield 94 g. II, m. 294°. β-(3,4-Methylenedioxyphenyl)-α-thiopyruvic acid (III), was prepared by suspending 108 g. II in 620 ml. 15% NaOH, heating on the water bath with occasional stirring until solution was complete, filtering, cooling to -5°, and adding 670 ml. 10% HCl. After 1 hr. at -5°, filtering and washing with H2O, and drying in vacuo, III was obtained in quant. yield (crude), m. 221-5° (decomposition) (AcOH-H2O). β-(3,4-Methylenedioxyphenyl)pyruvic acid oxime (IV) was obtained when 84 g. NH2OH.HCl in concentrated aqueous solution was poured into a solution of 27.5g. Na in 800 ml. EtOH, the NaCl filtered off, the filtrate added to 79.5 g. III, and warmed on the water bath until H2S evolution stopped. The solvent was evaporated in vacuo, the residue dissolved in 575 ml. 5% NaOH, filtered, cooled at 0°, and stirred with 600 ml. 10% HCl. The yellow, crystalline powder was filtered off, washed with water, and dried in vacuo over KOH to yield 76 g. (crude) IV, m. 159-61° (decomposition) (dilute EtOH). Homopiperonylic acid (V) was obtained when 62 g. IV was suspended in 240 ml. Ac2O, warmed carefully under reflux to completion of the reaction, and 15 min. further to boiling, and the excess Ac2O removed in vacuo to produce V nitrile, a red-brown oil, which was immediately saponified with 42 g. KOH in 75 ml. H2O and 300 ml. MeOH for 6 hrs. to give 28.5 g. V, m. 126-8°. V (24.8 g.) treated with 22 g. Br in 150 ml. glacial AcOH gave 35.9 g. 6-bromohomopiperonylic acid (VI), m. 190-1°. VI (27.5 g.), 15.1 g. o-nitrobenzaldehyde, 11.0 g. NEt3, and 100 ml. Ac2O heated 6 hrs. at 100° gave 32.3 g. α-(3,4-methylenedioxy-6-bromophenyl)-2-nitrocinnamic acid (VII), m. 238-9° (EtOH). VII (32.3 g.) in 300 ml. H2O and 80 ml. concentrated NH4OH was reduced in a mixture of 200 g. FeSO4.7H2O, 380 ml. H2O, and 140 ml. concentrated NH4OH to 26.2 g. VII 2-NH2

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analog (VIII), citron-yellow, m. 226-7° (decompn.) (EtOH). VIII (26.2 g.) in 300 ml. dioxane was treated with cooling and vigorous stirring with 6 ml. concd. H2SO4 and 12 ml. iso-AmONO, stirred 30 min., and the ppt. dissolved in 100 ml. H2O; 150 ml. 50% H3PO2 was quickly added, the soln. stirred, and poured into 1 l. H2O. The ppt. was filtered off, boiled with dil. Na2CO3 soln., filtered, acidified, and the ppt. filtered off and recrystd. several times from glacial AcOH to yield 9.6 g. 1-bromo-3,4-methylenedioxyphenanthrene-10-carboxylic acid (IX), m. 233-5° (decompn.). IX (8.0 g.) in 25 g. KOH and 350 ml. 50% EtOH was heated to boiling and 9 g. Zn dust added. After boiling 3 hrs., filtering, evapg. EtOH, acidifying with 1:1 HCl, filtering, and washing with H2O, the yellow ppt. was dried in vacuo at 110° to yield 6.2 g. 3,4-methylenedioxyphenanthrene-10-carboxylic acid (X), after vacuum sublimation at 150°, m. 274-5°, also prepd. by Pschorr ring closure of VIII; X with CH2N2 gave X Me ester (XI), m. 126° (MeOH). XI (900 mg.) and 5.1 ml. N2H4.H2O in 10 ml. dioxane and 20 ml. MeOH boiled 3 hrs. gave X hydrazide (XII), m. 248-52° (MeOH). XII (700 mg.) was dissolved in 20 ml. dioxane with warming, then cooled in ice water, and treated with 3.5 ml. concd. HCl, and then with 0.4 ml. iso-AmONO to give X azide (XIII), m. 91° (decompn.). XIII (475 mg.) boiled 3 hrs. in toluene freshly distd. over Na gave 3,4-methylenedioxy-10-phenanthryl isocyanate (XIV), not isolated, but boiled 1 hr. with 1 ml. Ac2O, then evapd. in vacuo, the residue dissolved in C6H6, heated with C, filtered, and treated with petr. ether until the turbidity disappeared. On cooling, 170 mg. of a mixt. sepd., m. 174-81°. The mixt. was distd. at 180°/0.001 mm. and the yellow oil crystd. several times from MeOH to give a substance, m. 255-6°, not identified. The MeOH soln. was evapd., and the residue again distd. at 180°/0.001 mm. to yield after two sublimations, 5 mg. 3,4-methylenedioxy-10-acetamidophenanthrene (XV), m. 274° which gave no m.p. depression when mixed with I. A stirred mixt. of 648 mg. X, 2 ml. CF3CO2H, and 2 ml. (CF3CO)2O, was treated with abs. CHCl3 until the soln. was clear, then with 200 mg. NaN3 to form a jelly, which was dild. with 20 ml. petr. ether, filtered off, washed with petr. ether, and dried in vacuo. The product was boiled with Et2O and evapd. to dryness quickly under N. The residue (XVI) (35 mg.), after distn. at 130°/0.001 mm., m. 153-4°, and was believed to be the amine from XV. The amine (XVII) obtained directly from I m. 154-5°. Both XVI and XVII, when diazotized, gave a violet-brown dye with alk. β-naphthol soln. XVI (20 mg.) in 2 ml. Ac2O, boiled 5 min. gave 11 mg. N-Ac compd., m. 274-5° (as did XV), no m.p. depression with I, m. 274°. The ultraviolet spectra were [location of max. in λ (log ε)]: I, 248 (4.61), 281 (3.91), 297 (3.72), 313 (3.87), 323 (3.85), 350 (3.34), 368 (3.30); XV, 248 (4.54), 282 (4.05), 298 (3.77), 314 (3.95), 324 (3.94), 350 (3.42), 368 (3.39). The infrared spectra of both I and XV in perfluorokerosine suspension gave a strong band at 3220 cm.-1, indicating the NH group, and thus the monoacetylamino group. V (4.5 g.), 3.8 g. o-nitrobenzaldehyde (XVIII), 2.5 g. NEt3, and 25 g. Ac2O heated 6 hrs. at 100°, treated carefully with 100 ml. H2O with addnl. warming, and cooled gave a resinous product, from which the liquid was

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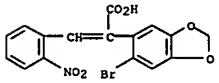
decanted. The resin was dissolved in NH4OH, filtered, acidified with 1:1 HCl with stirring, the crude acid filtered off, washed with H2O, and crystd. from AcOH to yield 4.6 g. α-(3,4-methylenedioxyphenyl)-2-nitrocinnamic acid (XIX), yellow crystals, m. 226-8° (EtOH). XIX (4.2 g.) was heated with 70 ml. H2O and 10 ml. NH4OH soln., added with stirring to 30 g. FeSO4.7H2O, 20 ml. NH4OH soln., and 200 ml. H2O on the water bath, stirred 30 min., filtered, and washed with hot H2O to give 2.4 g. yellow α-(3,4-methylenedioxyphenyl)-2-aminocinnamic acid (XX), m. 209-10°. XX (2.3 g.) in 40 ml. dioxane cooled 1 ml. concd. H2SO4 then 2 ml. iso-AmONO added dropwise with stirring, stirred 30 min., treated with 10 ml. H2O, then added quickly to 20 ml. 50% H3PO2 + Cu powder gave a white flocculent ppt. The mixt., free from diazonium salt, was poured into 100 ml. H2O, filtered, the ppt. digested with 1% KOH, filtered, washed with H2O, and dried in vacuo at 110° to yield 2.2 g. of an acid mixt., which, boiled with AcOH, recrystd. several times from HCONMe2, and sublimed at 210°/0.001 mm. gave an unidentified acid (XXI), m. 328-9°. From the mother liquor crude X was sepd. From the filtrate an acid was obtained in small amt., m. 219-21°, not identified. XXI (50 mg.) suspended in 50 ml. boiling AcOH, treated with a soln. of 100 mg. Na2Cr2O7 in 1 ml. H2O and 10 ml. AcOH, poured into 200 ml. H2O, extd. with CHCl3, the CHCl3 soln. washed with H2O, 1% KOH, and H2O, dried with Na2SO4, and evapd. yielded a red mass which was distd. at 186°/0.001 mm. The dark red compd. crystd. twice from AcOH and sublimed several times gave 8 mg. 2,3-methylenedioxy-9,10-phenanthrenequinone (XXII), m. 253°. The acid XXI was thus 2,3-methylenedioxyphenanthrene-10-carboxylic acid. XXI (50 mg.) decarboxylated with 50 mg. naturkupfer C in 5 ml. freshly distd. quinoline at 220° yielded, after crystn. from MeOH and distn. at 100°/0.001 mm., 2,3-methylenedioxyphenanthrene, leaflets, m. 93-5°; picrate m. 152°.

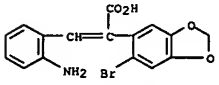
IT 131410-38-3P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)- 132569-41-6P, Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- 132727-17-4P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- 857176-14-8P, Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)-
RL: PREP (Preparation)
(preparation of)

RN 131410-38-3 CAPLUS
CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(o-nitrophenyl)- (6CI) (CA INDEX NAME)

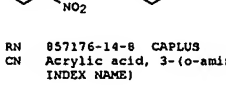


L4 ANSWER 235 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 132569-41-6 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 132727-17-4 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- (6CI) (CA INDEX NAME)



RN 857176-14-8 CAPLUS
CN Acrylic acid, 3-(o-aminophenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)

L4 ANSWER 236 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1959:50945 CAPLUS
DOCUMENT NUMBER: 53:50945
ORIGINAL REFERENCE NO.: 53:9129i,9130a-g
TITLE: Revision of structural assignments for geometrical isomers of 3-methyl-5-phenylpentadienoic acid
AUTHOR(S): Wiley, Richard H.
CORPORATE SOURCE: Imp. Coll. Sci. & Technol., London
SOURCE: Journal of the Chemical Society (1958) 3831-8
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Reinvestigation of the geometrical isomers of PhCH:CHCMe: CHCO2H (I) has shown that the compound, m. 125°, formerly assigned the cis-2-trans-4-structure is a mol. complex of the isomers, m. 158° and 160°. On the basis of their phys. properties and their infrared and ultraviolet absorption characteristics, these 2 isomers are now assigned the cis-2-trans-4- (Ia) and the trans-2-trans-4-structure (Ib), resp. This reassignment makes possible a new interpretation of the steric course of the Reformatskii reaction and of the mechanism of the decarboxylation by which the isomers are prepared, as well as the clarification of several inconsistencies and apparent abnormalities previously noted. In the Reformatskii reaction of PhCH:CHAc with BrCH2CO2Et the reaction was repeated on a 0.14-molal basis by the procedure previously given (Cawley and Nelan, C.A. 50, 4788i), giving a 1st fraction of 1.4 g. crystals, m. 124-52°, and 2.6 g., m. 124-6°. Recrystn. of the former gave Ib, m. 159-60°. The mol. complex purified by recrystn. from ligroine, or ligroine with 5% C6H6, m. 125-6°. Et senecioate and N-bromosuccinimide gave Me2CBrCH:CHCO2Et (II), n24D 1.4995. II by the Reformatskii reaction with BzH gave 15.14 g. unsatd. ester which was separated into 8 fractions, b3 115°/3 mm. to 166°/1.5 mm. The 7th fraction, b1.5 160-6°, was treated with saturated alc. KOH; acidification of the Et2O-extracted, diluted reaction mixture gave a solid which on recrystn. yielded 0.8 g. Ia, m. 158-8.5°. Further cooling of the mother liquor gave a 2nd and 3rd fraction. Recrystn. of the 2nd fraction gave 0.1 g. of the complex of Ia and Ib. The infrared spectra for 4 of the ester fractions showed a band at 1764 cm.-1, indicative of a γ-lactone. Attempts to isolate a γ-lactone by more careful fractionation were unsuccessful. Ia was obtained by the following procedure. The lutidine solution was not evaporated before being poured into dilute aqueous acid to precipitate the crude product.

HO2CC(:CHPh)CMe:CHCO2H (III) (7.10 g.) gave 3.55 g. Ia. III di-K salt warmed with AcOH and the Et2O solution of the neutral fraction evaporated gave a fraction, b3-5 76-81°, m. 33-5°, λ 218, 225, 232, and 282 mμ, ε 17,850, 17,400, 11,300, and 41,800, which may be PhCH:CHCMe:CH2. The infrared absorption spectrum shows a prominent band at 962 cm.-1, characteristic of the trans-disubstituted ethylenes. Either Ia or Ib, obtained by decarboxylation, or the mol. complex, when treated with iodine gave Ib. The mother liquors from the isomerization of Ib gave the mol. complex. Samples of Ib obtained from the iodine-catalyzed isomerization and Ib obtained by decarboxylation were used for the phase diagram. The 50% composition point is not a simple, single eutectic point. The existence of a maximum in the curve is not clearly shown by the available

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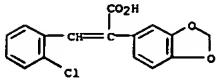
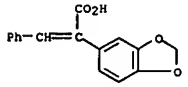
data. A mixt. of 0.6005 g. each of Ia and Ib fused together and recrystd.
gave the mol. complex, m. 125-6°. The infrared absorption spectrum for this sample is identical with, and superimposable on, that of the complex obtained from the Reformatskii reaction with benzylideneacetate. The complex may also be formed by recrystn. of equal amts. of Ia and Ib. Ia (0.93 g.) with CH2N2 in Et2O gave 0.67 g. of the Me ester (IV), m. 41.5-2.5° (ligroine), λ 232, 238, and 312 mμ, ε 14,350, 11,500, and 28,300. Similarly Ib (0.45 g.) with ethereal CH2N2 gave 0.41 g. Me ester (V), m. 35-6° (ligroine), λ 308, 238, and 232 mμ, 37,600, 9900, and 11,900. A mixt. of IV and V liquefied at room temp. Methylation of the mol. complex gave a mixt. of IV and V which, when cooled to -78°, pptd. crystals. The liquid residue, after thorough evacuation, was analyzed and had λ 310, 238, and 232 mμ, ε 32,000, 10,600, and 13,800. The infrared absorption spectra of the acids were detd. as Nujol mulls and those of the esters as liquid films.

IT 109697-83-8P, Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- 877169-81-8P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 109697-83-8 CAPLUS
CN Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 877169-81-8 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl- (6CI) (CA INDEX NAME)



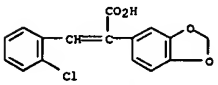
L4 ANSWER 237 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:50944 CAPLUS
DOCUMENT NUMBER: 53:50944
ORIGINAL REFERENCE NO.: 53:9129d-i
TITLE: The synthesis of α-(o-nitroaryl)cinnamic acids
AUTHOR(S): Pailer, M.; Schleppnik, A.; Meller, A.
SOURCE: Monatshefte fuer Chemie (1958), 89, 211-19
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The Perkin reaction of 1 mol. o- or p-nitroaryl acetic acids (I) with 1 mol. aromatic aldehyde was carried out in good yields in 1000 ml. Ac2O (II) 24 hrs. at the low temperature of 50-60° in the presence of 1.1 mols. Et3N as catalyst to give α-aryl cinnamic acids as intermediates for 3-arylidenoxindoles and phenanthrene carboxylic acids. The low reactivity of I in the Perkin reaction previously reported results from the ease of decarboxylation at higher temps. and is also a consequence of the mesomeric and inductive effects of the substituents on the acid and carbonyl reactants. The products were isolated from the condensation reaction by (A): adding 2-3 vols. H2O, boiling, cooling, decanting the H2O, digesting the oil or resin in dilute NH4OH on the steam bath, decolorizing with animal C, acidifying the filtrate with 5N HCl and recrystg. the precipitated nitrocinnamic acid; (B): adding 2-3 vols. cold H2O to decompose II and recrystg. the condensation product. With o-O2NC6H4CH2CO2H (III) (aldehyde, isolation method, yield and m.p. given): PhCHO (IV), A, 42, 193-4° (alc.); p-MeC6H4CHO, B, 37, 187° (HOAc); MeOC6H4CHO (V), A, 42, 172-3° (MeOH); (MeO)2C6H3CHO, A, 40, 158-9° (C6H6); piperonal (VI), A, 27, 226-7° (MeOH); 6-allylpiperonal, A, 25, 211-12° (HOAc); vanillin, B, 12, 196-7° (alc.); o-vanillin, B, 23, 204-5° (HOAc); o-HOC6H4CHO (VII), B, 32, α-(o-O2NC6H4)-2-acetoxy-3-methoxycinnamic acid 176-7° (HOAc); o-ClC2H4CHO (VIII), B, 77, 3-(2-nitrophenyl)-coumarin, 225° (HOAc); p-ClC6H4CHO, B, 70, 210-11° (HOAc); 6-bromopiperonal (IX), A, 55, 261-2° (HOAc) (at a reaction temperature of 30°, evolution of CO2 from decomposition of III and IX recovered unchanged); 6-bromoveratraldehyde, B, 57, 229-31° (HOAc); o-O2NC6H4CHO (X), A, 65, 207° (HOAc); m-O2NC6H4CHO, A, 96, 200-1° (alc.); 2,5-MeOO2NC6H3CHO, B, 38, 225-6°, (HOAc); 6-nitropiperonal, B, 78, 261° (HOAc); 2-nitroveratraldehyde, A, 68, 244° (HOAc); 6-nitroveratraldehyde, A, 66, 247° (HOAc); 3,4-(HO)2C6H3CHO, -, 0, -; 2,4-(OH)2C6H3CHO, -, 0, -; o-HO2CC6H4CHO, -, 0, -; p-Me2NC6H4CHO, -, 0, -. With p-O2NC6H4CH2CO2H: IV, A, 38, 225-6° (HOAc); V, B, 10, 244-5° (MeOH); X, A, 62, 185-6° (HOAc); VII, B, 26, 266-8°, (HOAc); VI, -, 0, -. With homopiperonylic acid (aldehyde and yield given): IV, 32; X, 62% (at a reaction temperature of 100°, 78% yield and at 125°, 38% yield); VIII, 51.

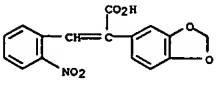
IT 109697-83-8P, Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- 132727-17-4P, Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- 877169-81-8P,

L4 ANSWER 237 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl-
RL: PREP (Preparation)
(prepn. of)

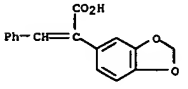
RN 109697-83-8 CAPLUS
CN Acrylic acid, 3-(o-chlorophenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 132727-17-4 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-(o-nitrophenyl)- (6CI) (CA INDEX NAME)



RN 877169-81-8 CAPLUS
CN Acrylic acid, 2-(3,4-methylenedioxyphenyl)-3-phenyl- (6CI) (CA INDEX NAME)

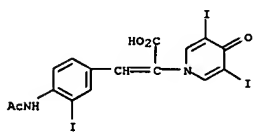


L4 ANSWER 238 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:2693 CAPLUS
DOCUMENT NUMBER: 53:2693
ORIGINAL REFERENCE NO.: 53:530d-g
TITLE: The relation between electrical resting potential of the isolated perfused mammalian muscle and the extracellular potassium concentration
AUTHOR(S): Pillat, B.; Kraupp, O.; Giebisch, G.; Stormann, H.
CORPORATE SOURCE: Univ. Vienna
SOURCE: Pfluegers Archiv fuer die Gesamte Physiologie des Menschen und der Tiere (1958), 266, 459-72
CODEN: AGPPAS; ISSN: 0365-267X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

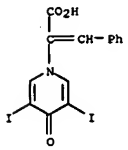
AB The resting potential (I) of the gracilus muscle, the mechanical tension (II) developed by the gastrocnemius muscle, the blood flow (III) and the lactic acid outflow (IV) of the isolated hindleg of the cat were determined, first with normal extracellular K concentration, then with increased K concentration, both at a constant product of K and Cl concentration (V) and at a constant Cl concentration At constant V the I was decreased by increased K concentration There was a linear relation between the decrease of I and the log of the K concentration At constant Cl concentration the same linear relation existed. The slopes of the two lines differed significantly. Both lines could be derived theoretically by assuming a Donnan equilibrium for K+ and Cl- on either side of the membrane. No changes in the II corresponding to the changes in the I could be found. Increase of the K concentration decreased the III strongly in both cases. A complete stop of the flow occurred at K concns. above 50 millimoles/l. No spontaneous increase of the IV occurred during the increase of the K concentration Due to the lowered III, the IV increased continually during the high K concentration

IT 101727-17-7P, 1(4H)-Pyridineacetic acid, α-(4-acetamido-3-iodobenzylidene)-3,5-diiodo-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 101727-17-7 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(4-acetamido-3-iodobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

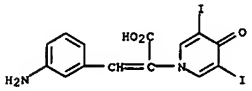


L4 ANSWER 239 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:61176 CAPLUS
DOCUMENT NUMBER: 52:61176
ORIGINAL REFERENCE NO.: 52:11037h-i,11038a
TITLE: α-[N-(3,5-Diiodo-4-pyridonyl)]cinnamic acids and their derivatives
AUTHOR(S): Bojarska-Dahlig, Halina
CORPORATE SOURCE: Inst. Farm., Warsaw
SOURCE: Roczniki Chemii (1957), 31, 1333-4
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A modified Perkin reaction between the respective aldehydes, Ac2O, and the Na salt of 3,5-diiodo-4-pyridone-N-acetic acid gave α-[N-(3,5-diiodo-4-pyridonyl)]cinnamic acid (I), m. 275-6°, and the following derivs. of I (m.ps. given): o-Cl (II), 251.5-2.5°; p-MeO (III), 271.5-3°; m-NO2 (IV), 276.5-8°, and p-NO2 (V), decompose IV and V were reduced to the corresponding NH2 derivs., (VI), m. 269.5-71°, and (VII), m. 263-4°, resp. Iodination of VI and VII with I2Cl in dilute HCl gave the respective amino iodocinnamic acids (VIII), m. 277.5-9.5°, and (IX), decompose 270°. III showed lowest toxicity in mice. Cholecystographic properties were studied on dogs and it was shown that I, VIII, and IX do not collect in the gall-bladder but are eliminated through the alimentary canal.
IT 100873-29-8, 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo-
(and derivs.)
RN 100873-29-8 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-benzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

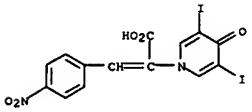


IT 100540-95-2P, 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- 100961-30-6P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- 106652-51-1P, 1(4H)-Pyridineacetic acid, α-[p-aminobenzylidene]-3,5-diiodo-4-oxo- 106652-68-0P, 1(4H)-Pyridineacetic acid, α-[m-aminobenzylidene]-3,5-diiodo-4-oxo- 106782-71-2P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-nitrobenzylidene-4-oxo- 106783-04-4P, 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-m-nitrobenzylidene-4-oxo-
RL: PREP (Preparation)

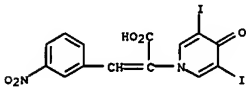
L4 ANSWER 239 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



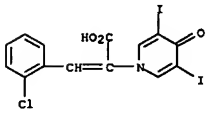
RN 106782-71-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(p-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



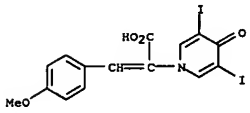
RN 106783-04-4 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-(m-nitrobenzylidene)-4-oxo- (6CI) (CA INDEX NAME)



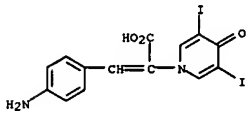
L4 ANSWER 239 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (prepn. of)
RN 100540-95-2 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-o-chlorobenzylidene-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



RN 100961-30-6 CAPLUS
CN 1(4H)-Pyridineacetic acid, 3,5-diiodo-α-p-methoxybenzylidene-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-51-1 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(p-aminobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)



RN 106652-68-0 CAPLUS
CN 1(4H)-Pyridineacetic acid, α-(m-aminobenzylidene)-3,5-diiodo-4-oxo- (6CI) (CA INDEX NAME)

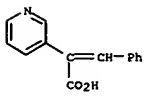
L4 ANSWER 240 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:55905 CAPLUS
DOCUMENT NUMBER: 52:55905
ORIGINAL REFERENCE NO.: 52:10078b-i,10079a-c
TITLE: N-Oxides and related compounds. VII. Peracid oxidation of some conjugated pyridines
AUTHOR(S): Katritzky, A. R.; Monro, A. M.
CORPORATE SOURCE: Oxford Univ., UK
SOURCE: Journal of the Chemical Society (1958) 150-3
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 52, 4633d. β-3- and β-4-Pyridylacrylic acids and their ethyl esters and amides, 2- and 4-styrylpyridines and pyridine-2-aldoxime and its semicarbazone gave 1-oxides with AcO2H. Pyridine (0.01 mole), 1.47 ml. 30% aqueous H2O2, and 6 ml. AcOH was heated 18 hrs. at 70°, volatile matter removed at 100°/15 mm., the residue either crystallized directly, or if semisolid treated in 15 ml. hot CHCl3 with 0.8 g. K2CO3 and recovered from the CHCl3 by evaporation The following 1-oxides were prepared: β-4-pyridylacrylic, prisms, m. 237-40° (AmOH) (decomposition), hemiacetate, plates, m. 237-40° (AcOH) (decomposition); β-4-pyridylacrylamide, prisms, m. 246° (MeOH or H2O) (decomposition); Et β-4-pyridylacrylate, prisms, m. 145° (C6H6-petr. ether), which with 2N aqueous NaOH during 12 hrs. at 100° followed by AcOH gave the corresponding acid, m. 238-40° (decomposition), and with aqueous methanolic NH3 in 5 days at 0° gave the amide, m. 245° (decomposition); β-3-pyridylacrylic acid, prisms m. 273-4° (AcOH) (decomposition); β-3-pyridylacrylamide, needles, m. 235° (EtOH-H2O) (decomposition); Et β-3-pyridylacrylate, prisms, m. 99-101° (AcOEt), also prepared by esterification of the corresponding acid with EtOH-H2SO4, converted (as in the 4-series) into the acid, m. 274-5° (decomposition), and the amide, m. 235° (decomposition). Oxidation gave the oxide of the 2-isomer as prisms, m. 162° (C6H6), and the 4-isomer gave an oxide, prisms, m. 169° (MeCOEt). BzH (10.6 g.), 10.9 g. 2-picoline 1-oxide, and 50 ml. 5% KOMe in MeOH was refluxed 3 hrs., after 12 hrs. more, excess CO2 was passed in, the whole filtered and steam distilled yielding 22% 2-styrylpyridine 1-oxide, m. 160°. 4-Picoline 1-oxide similarly gave 11% 4-styrylpyridine 1-oxide, m. 167-9°. Refluxing 20.4 g. Et 3-pyridylacetate 8 hrs. with 11 g. KOH in 11 ml. H2O and 28 ml. EtOH followed by addition of 14.6 ml. aqueous 12N HCl, filtration, evaporation, and extraction of the residue with MeOH gave 75% 3-pyridylacetic acid, m. 141-3°; 1-oxide, prisms, m. 142-4° (AcOEt-EtOH) (decomposition). The acid (1.27 g.), 1.5 ml. BzH, 0.2 ml. piperidine, and 10 ml. pyridine heated 2 days at 115° and poured into H2O gave 40% β-phenyl-α-3-pyridylacrylic acid, needles, m. 234-5° (EtOH) (decomposition). Aqueous 10% NaOH (0.5 ml.) was added slowly at 0° to 1.07 g. pyridine-2-aldehyde and 1.17 g. PhCH2CN in 2.0 ml. EtOH; after 18 hrs. 74% α-phenyl-β-2-pyridylacrylonitrile was collected as prisms, m. 63-6° (EtOH). O-Benzoyl(pyridine-2-aldehyde cyanohydrin), prepared as the oxime benzoate below, formed prisms, m. 102° (EtOH). Pyridoin, needles, m. 156°, separated later from the aqueous mother liquors. Aqueous NaCN (0.94 g. in 2 ml.) was added slowly at -10° to 3.14 g. quinoline-2-aldehyde in 10 ml. aqueous 2N HCl and the precipitated solid recrystd. (C6H6 and AcOEt) to

L4 ANSWER 240 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
give 62% 1-cyano-1,2-di(2-quinolyl)-ethane-1,2-diol, brown plates, m. 133° (decompn.). v Oxidation gave the aldoxime oxide, needles, m. 222° (EtOH) (decompn.); semicarbazone oxide, insol. in CHCl3, needles, m. 233° (AcOH-AcOEt) (decompn.). Both compds. with 2,4-dinitrophenylhydrazine in alc. HCl gave the corresponding 2,4-dinitrophenylhydrazone 1-oxide, needles, m. 285-90° (AcOH) (decompn.). Extn. of crude pyridine-2-aldehyde cis-semicarbazone 1-oxide with CHCl3 gave (from the CHCl3) 3% cis-semicarbazone, prisms, m. 158° (EtOH). On treatment with alc. HCl and 2,4-dinitrophenylhydrazine, both the cis- and normal semicarbazones gave the 2,4-dinitrophenylhydrazone, m. 226-8°. BzCl (0.32 ml.) was added slowly to 0.31 g. pyridine-2-aldoxime in 1 ml. pyridine at 0°, the mixt. kept 18 hrs., and H2O added yielding 80% O-benzoyl(pyridine-2-aldoxime), prisms, m. 85-90° (EtOH). Treatment with AcO2H gave BzOH and pyridoin, m. 152°. 4-Acetylpyridine gave the azine, plates, m. 125.5-7° (petr. ether), and when heated 1 min. with 2 parts hydrazine hydrate yielded the hydrazone, plates, m. 121-2° (C6H6). Oxidation of 2-, 3-, and
4-(N'-benzenesulfonylhydrazinocarbonyl)p
yridine gave the 4-substituted pyridine 1-oxide, needles, m. 238-9° (H2O) (decompn.), the 3-analog, needles, m. 222-4° (H2O or EtOH) (decompn.), and the 2-analog, needles, m. 209-12° (AcOH) (decompn.). Et isonicotinate (5.5 g.) was refluxed 4 hrs. with 12 ml. PhCH2NH2 and excess amine removed at 100°/14 mm. yielding 71% N-benzylisonicotinamide, needles, m. 90-2° (AcOEt-petr. ether); the methotoluene-p-sulfonate formed plates, m. 194.5-6.5° (EtOH). N-2-(3-Indoyl)ethylisonicotinamide, m. 165.5-67°, was similarly prepd. by heating the amine and ester for 10 hrs. at 140° and sepg. from EtOH-C6H6; methotoluene-p-sulfonate, plates, m. 174-5.5° (AcOEt-EtOH). Oxidation gave pure β-4-pyridylpropionamide 1-oxide, rods, m. 227° (EtOH), and N-benzylisonicotinamide 1-oxide, prisms, m. 184° (EtOH).

IT 32967-19-4P, 3-Pyridineacetic acid, α-benzylidene-
RL: PREP (Preparation)
(preparation of)

RN 32967-19-4 CAPLUS

CN 3-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)



L4 ANSWER 241 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:35138 CAPLUS
DOCUMENT NUMBER: 52:35138
ORIGINAL REFERENCE NO.: 52:6298f-i,6299a-b
TITLE: Synthesis of 1-methoxy-5,6-methylenedioxyphenanthrene
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi; Toyonaka, Keiko
CORPORATE SOURCE: Nagoya City Univ. Pharm. School
SOURCE: Nagoya-shiritsu Daigaku Yakugakubu Kiyo (1957), 5, 58-60
CODEN: NADYAS; ISSN: 0469-4805
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

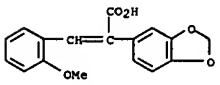
AB Na 6-bromohomopiperonylate, 2.2 g. 2-methoxy-6-nitrobenzaldehyde, and 20 cc. Ac2O is heated at 120° 32 hrs., 40 cc. H2O added, heated on a steam bath 30 min., the AcOH vacuum distilled, 200 cc. 5% NH4OH added, filtered, the filtrate shaken with ether to remove impurities, acidified with HCl, extracted with EtOAc, and the product recrystd. from MeOH to afford
3.2 g. 2-methoxy-6-nitro-α-(3,4-methylenedioxy-6-bromophenyl)cinnamic acid (I), light yellow columns, m. 260-1° (decomposition). I (1.5 g.) in 15 cc. 5% NH4OH is added dropwise to 9 g. FeSO4, 22 cc. H2O, and 20 cc. concentrated NH4OH with shaking, warmed on a steam
bath 20 min., filtered, the filtrate adjusted to pH 5.0 by dilute HCl, and
the precipitate recrystd. from C6H6 to afford 1.0 g. 2-methoxy-6-amino-α-
(3,4-methylenedioxy-6-bromophenyl)cinnamic acid (II), light yellow needles, m. 202-3°. To 0.3 g. II in 7 cc. MeOH is added 4.3 cc. 20% H2SO4, cooled at 0°, diazotized with 3 cc. N NaNO2 solution, kept 30 min., 3 cc. H2O added, 0.3 g. Gatterman's mol. Cu added with shaking, heated on a steam bath 1 hr., made alkaline by NH4OH, the Cu removed, the filtrate evaporated in vacuo, acidified with HCl, the precipitate extracted with ether,
and recrystd. from MeOH to afford 0.06 g. 1-bromo-3,4-methylenedioxy-8-methoxyphenanthrene-10-carboxylic acid (III), m. 265-85°. III (0.06 g.) in 60 cc. alc. is reduced using 30 cc. 10% KOH-alc. and 0.2 g. Pd-C as catalyst, evaporated in vacuo, dissolved in 15 cc. H2O, acidified with
HCl, extracted with ether, and recrystd. from MeOH to afford 0.04 g. 1-methoxy-5,6-methylenedioxyphenanthrene-9-carboxylic acid (IV), light yellow needles, m. 269-70°. IV (0.04 g.) and 0.2 g. Gatterman's mol. Cu in 5 cc. quinoline is heated at 180-200° 10 min., then boiled 250-60° 20 min., cooled, diluted with ether, Cu removed, the ether layer shaken with dilute HCl to remove quinoline, shaken with 2% NaOH
solution to remove unreacted IV, the ether evaporated, the residue dissolved in
C6H6, chromatographed on an alumina column, and recrystd. from MeOH to afford 0.01 g. 1-methoxy-6,6-methylenedioxyphenanthrene (V), columns, m. 87-8°; picrate, reddish brown needles from alc., m. 180° (decomposition). 2-Methoxy-α-(3,4-methylenedioxyphenyl)cinnamic acid (VI) was also prepared Na homopiperonylate (0.5 g.) and o-methoxybenzaldehyde in 5 cc. Ac2O is heated at 110-20° 10 hrs., 10 cc. H2O added, heated on a steam bath 30 min., the AcOH evaporated in

L4 ANSWER 241 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
vacuo, 30 cc. 5% NH4OH added, filtered, the filtrate shaken with ether to remove the unreacted compds., acidified with HCl, and recrystd. from dil. AcOH to afford 0.9 g. VI, light yellow needles, m. 219-20°.

IT 87751-89-1P, Acrylic acid, 3-(o-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- 111089-64-6P, Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)-130862-09-8P, Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)-
RL: PREP (Preparation)
(preparation of)

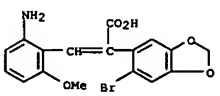
RN 87751-89-1 CAPLUS

CN 1,3-Benzodioxole-5-acetic acid, α-[(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



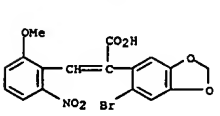
RN 111089-64-6 CAPLUS

CN Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(2-bromo-4,5-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)



RN 130862-09-8 CAPLUS

CN Acrylic acid, 2-(2-bromo-4,5-methylenedioxyphenyl)-3-(2-methoxy-6-nitrophenyl)- (6CI) (CA INDEX NAME)



L4 ANSWER 242 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:51904 CAPLUS
DOCUMENT NUMBER: 51:51904
ORIGINAL REFERENCE NO.: 51:9646b-f
TITLE: Alkaloids of menispermaceous plants. CXLIII. Alkaloids
of Stephania capitata. 5
AUTHOR(S): Shirai, Hideaki; Oda, Noriichi
CORPORATE SOURCE: Nagoya City Univ.
SOURCE: Yakugaku Zasshi (1956), 76, 1287-9
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

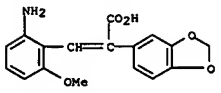
AB cf. C.A. 46, 125d; 51, 1542i. A mixture of 5 g. 3,4-CH2O2C6H3CH2CO2 Na, 4.5
g. 2,6-MeO(O2N)C6H3CHO, and 25 ml. Ac2O heated 20 hrs. at 110-20°, the product boiled with 50 ml. H2O, the AcOH removed in vacuo, the residue
in 300 ml. 5% NH4OH filtered, the filtrate washed with Et2O, the aqueous layer
acidified with HCl, the precipitate taken up in AcOEt, the AcOEt removed, and the
residue recrystd. from MeOH gave 4.5 g. 2,6-MeO(O2N) C6H3CH:C(C6H3O2CH2-3,4)CO2H (I), needles, m. 206-7°; 4.4 g. FeSO4 in 10 ml. H2O and 12 ml. NH4OH treated dropwise with 1 g. I in 20 ml. 5% NH4OH, heated 10 min. at 100°, the solution filtered, and the filtrate treated with HCl to pH 5 gave 0.8 g. 6-NH2 analog (II) of I, m. 107-9° (decomposition); recrystn. of II in MeOH converted into 5-methoxy-3-(3,4-methylenedioxyphenyl)carbostyril, needles, m. 267-8°; 2 g. II in 40 ml. MeOH and 25 ml. 20% H2SO4 at 0° treated dropwise with 20 ml. 1N NaNO2, let stand 30 min., 30 ml. H2O added, heated 30 min. with 10 g. Cu, the solution made alkaline with NH4OH, the Cu and MeOH removed, and the residue
extracted with Et2O gave 0.2 g. 1-methoxy-6,7-methylenedioxyphenanthrene-9-
carboxylic acid (III), light yellow needles, m. 300-1° (decomposition), and the mother liquor concentrated gave 0.15 g. 5,6-CH2O2 analog (IV) of III, m.
267-8°; 0.15 g. IV in 10 ml. C9H7N heated 10 min. with 0.5 g. Cu at 180-200° and 20 min. at 250-60, the solution filtered, the filtrate with Et2O washed with dilute HCl and NaOH, the oil b0.1 210-20° further purified through Al2O3 gave 0.03 g. 1-methoxy-5,6-methylenedioxyphenanthrene (V), columns, m. 86-7° (picrate, m. 180° (decomposition)). Similarly, III yielded 1-methoxy-6,7-methylenedioxyphenanthrene, prisms, m. 150°; picrate, m. 192-3°(decomposition). Thus, the structure of stephane is confirmed to be 1-methoxy-5,6-methylenedioxyaporphine.

IT 110394-33-7P, Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- 111529-61-4P, Acrylic acid, 3-(2-methoxy-6-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-
RL: PREP (Preparation)
(preparation of)

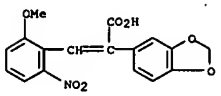
RN 110394-33-7 CAPLUS

CN Acrylic acid, 3-(2-amino-6-methoxyphenyl)-2-(3,4-methylenedioxyphenyl)- (6CI) (CA INDEX NAME)

L4 ANSWER 242 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



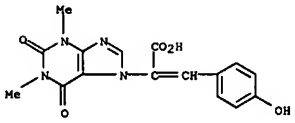
RN 111529-61-4 CAPLUS
CN Acrylic acid, 3-(2-methoxy-6-nitrophenyl)-2-(3,4-methylenedioxyphenyl)-(6CI) (CA INDEX NAME)



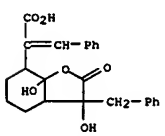
L4 ANSWER 243 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:9499 CAPLUS
DOCUMENT NUMBER: 51:9499
ORIGINAL REFERENCE NO.: 51:2025f-h
TITLE: 7-Theophyllineacetic acid derivatives
INVENTOR(S): Schlesinger, Albert; Weiner, Nathan; Gordon, Samuel M.
PATENT ASSIGNEE(S): Endo Laboratories Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2712016		19550628	US 1952-292194	19520606

AB [Y in this abstract = 7-theophyllinyl]. The Na salt of 7-theophyllineacetic acid (416 g.) (anhydrous), 1200 g. Ac2O, and 192 g. HOC6H4CHO refluxed with stirring about 24 hrs. at 110-12°, the Ac2O and AcOH evaporated in vacuo, the residue stirred with 800 g. H2O and 100 g. ice until it dissolves, 40% NaOH added until alkaline to phenolphthalein, then 200 ml. excess, the mixture heated to 65° with stirring on a water bath, held at room temperature 2 hrs., filtered through glass wool, and the filtrate poured into 2200 concentrated HCl and 2000 g. ice and kept 24 hrs. in an ice bath ppts. 54% YC(:CHR)CO2H (R = p-HOC6H4), m. 254° (from boiling EtOH). By use of the appropriate materials were prepared 94% YCHRCO2H (R = p-HOC6H4CH2), m. 170°; 86% YCHRCO2H [R = 3,5,4-I2(HO)C6H2CH2] (I), m. 274° (from AcOH); the Na salt of I; and the piperidine salt of I, m. 189°. These derivs. are valuable as bactericides, amebicides, and x-ray contrast agents.
IT 101352-23-2P, Purine-7-acetic acid, 1,2,3,6-tetrahydro-α-p-hydroxybenzylidene-1,3-dimethyl-2,6-dioxo-
RL: PREP (Preparation)
(preparation of)
RN 101352-23-2 CAPLUS
CN Purine-7-acetic acid, 1,2,3,6-tetrahydro-α-p-hydroxybenzylidene-1,3-dimethyl-2,6-dioxo- (6CI) (CA INDEX NAME)



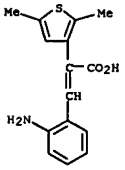
L4 ANSWER 244 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:82002 CAPLUS
DOCUMENT NUMBER: 50:82002
ORIGINAL REFERENCE NO.: 50:15497h-i,15498a-c
TITLE: The condensation of cyclohexanone with phenylpyruvic acid
AUTHOR(S): Kristensen, Johan; Cordier, Paul
SOURCE: Compt. rend. (1956), 242, 908-10
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Aqueous Na-phenylpyruvate (I) with an equimolar amount of cyclohexanone (II) in 3% KOH at 0° for 8 days, then addition of ether, gives 28% of 22,62-diphenyl-21,61-dihydroxy-21,61-dicarboxy-2,6-diethylcyclohexanone (III), m. 285° (semicarbazone, m. 254°; dinitrophenylhydrazone, m. 226°), when purified in HOAc. The ether extract contains 15% of 22-phenyl-21-hydroxy-21-carboxy-2-ethylcyclohexanone (IV), m. 127° obtained by extraction with KHCO3 solution, precipitation with acid, extraction into ether and solvent evaporated, and the crystals triturated with cold C6H6. III and IV decompose in aqueous base to I and II. A large excess of II doubles the yield of IV. III with HCl in HOAc at 100° gives an ethylenic monoacid, m. 118°, possibly V, which gives BzH (VI) with MnO4-and VI and I with hot NaOH. Cold concentrated H2SO4 with III gives the corresponding β-diketone, m. 90°, with loss of H2O and CO. Cold H2SO4 with 1/3 HOAc and III gives the diethylenic diacid, m. 181°, and MnO4- with this compound gives VI and an α,γ-diketo acid. IV with HCl in HOAc at 100° gives VII, m. 91°, and a corresponding ethylenic acid, m. 98°, also obtained with cold H2SO4 and 1/3 HOAc. IV with concentrated H2SO4 gives 1,2,3,4-tetrahydrophenanthrene-10-carboxylic acid, m. 210°. V with KBH4 gives the α,γ-dihydroxy acid, m. 184°, and the corresponding lactone, m. 164°; Raney Ni hydrogenation gives an isomeric lactone, m. 121°. III fails to hydrogenate. A similar condensation with o-methylcyclohexanone (with alc. present) gives only the α-hydroxy-γ-oxo acid, m. 154°.
IT 858791-52-3P, 7-Benzofuranacetic acid, 3-benzyl-α-benzylideneoctahydro-3,7a-dihydroxy-2-oxo-
RL: PREP (Preparation)
(preparation of)
RN 858791-52-3 CAPLUS
CN 7-Benzofuranacetic acid, 3-benzyl-α-benzylideneoctahydro-3,7a-dihydroxy-2-oxo- (5CI) (CA INDEX NAME)



L4 ANSWER 244 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

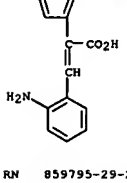
L4 ANSWER 245 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1955:23854 CAPLUS
DOCUMENT NUMBER: 49:23854
ORIGINAL REFERENCE NO.: 49:4619c-i,4620a-b
TITLE: Polynuclear thiophenes. III. 1,3-Dimethyl-4,5-benzisothianaphthene
AUTHOR(S): Dann, Otto; Distler, Harry
CORPORATE SOURCE: Univ. Erlangen, Germany
SOURCE: Chemische Berichte (1954), 87, 365-73
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 49, 1696h. After a discussion of the chemical, phys., and biol. properties of thiophene, naphthalene, and benzene derivs. the preparation of 1,3-dimethyl-4,5-benzisothianaphthene (I) is described and its properties are compared with those of 9,10-dimethyl-1,2-benzanthracene (II). Heating 10 g. 2,5-dimethyl-3-acetylthiophene, 18 cc. dioxane, 22 cc. concentrated NH4OH, 15 g. S, and 12 cc. yellow (NH4)2Sx in a bomb tube 4 hrs. at 160° and evaporating the mixture on a water bath to dryness give 70% (2,5-dimethyl-3-thienyl)acetamide (III), m. 147-8°. Refluxing 10 g. III with 10 g. KOH in 100 cc. MeOH and 5 cc. H2O 12 hrs. gives 54% free acid (IV), m. 68-70°. When 12.7 g. o-O2NC6H4CHO and 12 g. Na salt of IV (dried 6 hrs. at 130°) are refluxed 7 hrs. at 160-70° with 2 g. ZnCl2 in 140 cc. Ac2O, 100 cc. H2O is added carefully to the hot mixture, and the latter is poured into 1 l. H2O 62% 2-nitro-α-(2,5-dimethyl-3-thienyl)cinnamic acid (V), yellow crystals, m. 196°, is obtained. Adding 250 cc. concentrated NH4OH to 110 g. Fe(NH4)2(SO4)2.6H2O in 750 cc. H2O, then adding 10.3 g. V in 100 cc. 10% NH4OH, boiling the mixture 2 hrs. with stirring, and adjusting the filtered solution to pH 5 give 66% 2-NH2 analog (VI) of V, fine needles, m. 215-17°. Adding with stirring 30 g. VI in 400 cc. H2O containing 20 g. KOH to 800 cc. H2O containing 70 cc. H2SO4, then adding (1 hr.) at 0° 25 g. NaNO2 in 150 cc. H2O, stirring the mixture another 4 hrs. at 0-3°, destroying the excess NaNO2 by the addition of 25 g. H2NSO3H in 200 cc. H2O, stirring the solution 5 hrs. with Cu paste [prepared according to Gatterman [Ber. 23, 1219(1890)] from 250 g. crystalline CuSO4], keeping it overnight, filtering off the precipitate, extracting it with dilute NaOH, and acidifying the alkaline solution with dilute H2SO4 give 60-5% crude 1,3-dimethyl-4,5-benzisothianaphthene-7-carboxylic acid (VII) [Me ester (CH2N2), golden-yellow leaflets, m. 226-7° (sealed tube)]. The extracted precipitate is dried overnight at 70°, mixed with some "Naturkupfer C," divided into 3 parts, and each part (about 30 g.) added in 2-3 g. batches to 100 cc. quinoline at 210-20°. The mixture is then heated a very short time to 230° and, after cooling to about

L4 ANSWER 245 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
180°, is poured very slowly into 1 l. H2O contg. 100 cc. concd. H2SO4. The ppt. formed is washed exhaustively with dil. H2SO4 and H2O, suspended in 200 cc. warm Me2CO, 1 l. benzine added to the filtered soln., the amorphous ppt. formed is discarded, the filtered soln. washed (1% H2SO4, 1% NaOH, and H2O), and the dried benzine soln. passed through an Al2O3 column. The yellow zone is eluted with 2 l. benzine (b. 60-70°), the residue of the benzine soln. distd. at 135-40°/4 mm., and the distillate treated in abs. EtOH with picric acid in EtOH, giving I picrate, dark red-brown needles, m. 148-9°, which, decompd. in ether with NaOH and the residue of the ether distd. at 0.4 mm., gives 4% I, needles, m. 82.5-3°. Refluxing 1 g. I in 25 cc. Me2CO with 10 g. maleic anhydride (VIII), pouring the mixt. into 250 cc. H2O contg. 2 g. NaOH, and extg. with ether give 1,4-dimethyl-1,4-endothio-1,2,3,4-tetrahydrophenanthrene-2,3-dicarboxylic anhydride, m. 169-70°, which is also obtained when 50 mg. I and 500 mg. VIII are fused at 160°. Heating 10 g. V mixed with 1 g. Cu chromite in 30 cc. quinoline 0.5 hr. at 230°, pouring the mixt. into dil. H2SO4, extg. with ether, and distg. the residue of the ext. at 205-12°/1.5 mm. give β-(2,5-dimethyl-3-thienyl)-2-nitrostyrene (IX), m. 98-9°. Refluxing 2 g. IX in 25 cc. AcOH and 15 cc. concd. HCl 2 hrs. with 5 g. granulated Zn, distg. the reaction product at 120-60°/0.4 mm., and treating the distillate with HCl give β-(2,5-dimethyl-3-thienyl)-2-aminostyrene-HCl, m. 191-2° (picrate, m. 159-60°). Distg. 60 g. 2-thienylacetamide and 65 g. P2O5 at 216-20° gives 45% 2-thienylacetonitrile (X), b12 105-10°, nD22 1.5436. Refluxing 10 g. X and 20 g. p-MeC6H4SO3H.H2NCH2CH2NH2 1.5 hrs. at 200°, adding dil. NaOH, extg. with CHCl3, and distg. the residue of the CHCl3 ext. give 2-(2-thienylmethyl)imidazoline, b3 166-7°, needles, m. 64-5° (picrate, m. 229-30°).
IT 853919-12-7P, 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl-, hydrochloride 853919-13-8P, 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl- 859795-29-2P, 3-Thiopheneacetic acid, 2,5-dimethyl-α-o-nitrobenzylidene-
RL: PREP (Preparation)
(preparation of)
RN 853919-12-7 CAPLUS
CN 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl-, hydrochloride (5CI) (CA INDEX NAME)

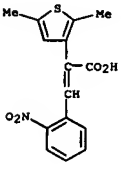


● HCl

RN 853919-13-8 CAPLUS
CN 3-Thiopheneacetic acid, α-(o-aminobenzylidene)-2,5-dimethyl- (5CI) (CA INDEX NAME)

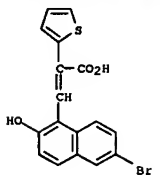


RN 859795-29-2 CAPLUS
CN 3-Thiopheneacetic acid, 2,5-dimethyl-α-o-nitrobenzylidene- (5CI) (CA INDEX NAME)



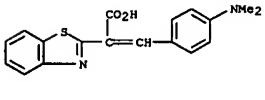
L4 ANSWER 246 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1954:18264 CAPLUS
DOCUMENT NUMBER: 48:18264
ORIGINAL REFERENCE NO.: 48:3327i,3328a-c
TITLE: Derivatives of 6-bromo-2-methoxy-1-naphthaldehyde of biological interest
AUTHOR(S): Hoan, Nguyen
CORPORATE SOURCE: Pharm. fac., Paris
SOURCE: Bulletin de la Societe Chimique de France (1953) 309-14
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:18264
AB A series of 2,3-diarylacrylonitriles and 3-aryl-5,6-benzocoumarins derived from 6-bromo-2-methoxy-1-naphthaldehyde (I) are described. These compds. are being investigated as antagonists of sexual hormones and as inhibitors of plant auxins. I b15 234-40°, m. 110°, from 6,2-BrC10H6OMe, HCONHMe, and POCl3; semicarbazone, m. 246°; thiosemicarbazone (Ia), m. 240°. 6-Bromo-2-methoxy-1-styrylnaphthalene b15 275-80°, m. 101-40° (perhaps a mixture of cis and trans forms), from I and BzMgCl. 6-Bromo-2-methoxy-1-(2,4,6-trinitrostyryl)naphthalene m. 205°, from I and TNT. The following α-(6-Bromo-2-methoxy-1-naphthyl)-β-arylacrylonitriles were prepared (aryl and m.p. given): Ph 159°, p-tolyl 170°, p-EtC6H4 128°, p-ClC6H4, 161°, p-BrC6H4 190°, p-IC6H4 207°, p-O2NC6H4 226°, 2-thienyl 130°, 3-thianaphthenyl 165°. 3-Aryl-5,6-(3-bromobenzo)coumarins (3-aryl and m.p.): Ph 247°, p-tolyl 297°, p-EtC6H4 238°, p-ClC6H4 328°, p-BrC6H4 342°, p-IC6H4 350°, p-O2NC6H4 355°, 2-thienyl 242°, 3-thianaphthenyl 266°. Ia was treated with the following acids to give the corresponding I 4-oxo-2-thiazolin-2-ylhydrazone (II) substituted in the 5 position of the thiazoline nucleus (acid and m.p. of II given): monochloroacetic 305°, α-bromobutyric 229°, α-bromoisovalerianic 237°, α-bromolauric 188°,α-bromomyristic 195°, α-bromopalmitic 184°, α-bromostearic 171°, α-bromodihydrohydnocarpic 169°, α-bromodihydrochaulmoogric 181°.
IT 858200-16-5P, 1-Naphthaleneacrylic acid, 6-bromo-2-hydroxy-α-2-thienyl-, δ-lactone
RL: PREP (Preparation)
(preparation of)
RN 858200-16-5 CAPLUS
CN 1-Naphthaleneacrylic acid, 6-bromo-2-hydroxy-α-2-thienyl-, δ-lactone (5CI) (CA INDEX NAME)

L4 ANSWER 246 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 247 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1953:444 CAPLUS
DOCUMENT NUMBER: 47:444
ORIGINAL REFERENCE NO.: 47:57g-i,58g-i,59a-g
TITLE: Photographic α-substituted carbocyanine sensitizers
AUTHOR(S): van Dormael, A. E.; Nys, J.
SOURCE: Chimie et Industrie (Paris) (1950), 63(No. 3 bis), 483-8
CODEN: CHIEAN; ISSN: 0009-4358
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Benzothiazole (I), benzoselenazole, and benzoxazole derivs. having in the 2-position a CH2COA group, where A is OEt, NHPh, NH2, NHNH2, or NHN:CHPh, condense readily with aromatic aldehydes, and heterocyclic alkylthio and 2-anilinovinyl cyclammonium salts to yield styryl, cyanine, and carbocyanine dyes. Et 2-benzothiazoleacetate (II) is prepared from EtO2CCH2COCl (III) and (o-H2NC6H4S)2Zn in C6H6 (cf. Staudinger and Becker, C.A. 12, 696). Similarly is prepared from (o-H2NC6H4Se)2Zn and III, Et 2-benzoselenazoleacetate, colorless crystals, m. 61-2°. Et 2-benzoxazoleacetate, m. 65-6°, is obtained from its Ag salt and EtI in CHCl3. II and PhNH2 in xylene in the presence of a trace of pyridine give 2-benzothiazoleacetanilide (IV), colorless crystals, m. 161-1.5°. II and concentrated aqueous NH3 yield 2-benzothiazoleacetamide, m. 175-6° (from EtOH). 2-Benzothiazoleacethydrazide (V), m. 151-2° (from EtOH), is prepared from II and H2NNH2.H2O in EtOH. V and BzH give benzaldehyde 2-benzothiazoleacethydrazone, m. 180-1° (from C5H11OH). Condensation of II and IV with p-Me2NC6H4CHO (VI) yields Et α-(4-dimethylaminobenzylidene)-2-benzothiazoleacetate (VII), m. 149-50°, λmaximum 400 mμ, log ε 4.54, and α-(4-dimethylaminobenzylidene)-2-benzothiazoleacetanilide (VIII), m. 223-4°, λmaximum 408 mμ, log ε 4.72, resp. Equimol. quantities of V and VI form a white precipitate, presumably p-dimethylaminobenzaldehyde 2-benzothiazoleacethydrazone (IX), which is converted by a 2nd mol. VI to the α-(4-dimethylaminobenzylidene) derivative (X) of IX, yellow solid, m. 211-12°, λmaximum 402 mμ, log ε 4.74. Condensation of I derivs. with 2-methylthiobenzothiazolium-MeX in EtOH in the presence of Et3N gives the following XI (A, m.p., λmaximum, and log ε given in the indicated order): OEt (XII), m. 148-9°, 385.5 mμ, 4.32; NHPh, m. 185-7°, 398.0 mμ, 4.52; NH2, m. 181-1.5°; and NHN: CHPh, m. 267-8°, 390 mμ, 4.69. From I derivs. and 2-(2-anilinovinyl)-1-ethylbenzothiazolium-MeX in EtOH in the presence of Ac2O are obtained the following carbocyanines XIII (A given): OEt (XIV), m. 162-2.5°; NHPh (XV), m. 172-4°; and NHN:CHPh (XVI), m. 185-7°. II heated with MeI in a sealed tube gives the methiodide, m. 170-1° (decompose) (from Me2CO), which gives with VI in Ac2O VII-MeI, m. 143-5°. Similarly are prepared XII-EtI, m. 187-8°; and XIV-EtI, m. 215-16°. Condensation of II with HC(OEt)3 in Ac2O yields by cyclization of the intermediate condensation product XVII, m. 294-5°; shows a strong blue fluorescence. The presence of the α-substituent of the type CH2COA in XIII shifts the absorption maximum (given) towards longer wave lengths as compared to the

L4 ANSWER 247 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
unsubstituted compd. (XVIII): XIV 489.1 mμ, log ε 4.80; XV 493.5 mμ, log ε 4.83; XVI 500.0 mμ, log ε 4.86; and XVIII 455.0 mμ, log ε 4.71. In XVIII-EtX 2 limiting structures of equal energy content having the pos. charge on either one of the 2 N make main contributions to the resonance hybrid, the introduction of an α-carbonyl substituent as in XIV-EtX causes the appearance of a 3rd electromeric form which destroys the energetic symmetry of the mol. and causes a hypsochromic effect lowering the absorption max. from 560 mμ (log ε 5.25) for XVIII-EtX to 504 mμ (log ε 4.82) for XIV-EtX. A similar bathochromic effect for the XI or a hypsochromic effect for XII-EtI as compared with the unsubstituted compds. (λmax. 388.5 mμ, log ε 4.82, and λmax. 424 mμ, log ε 4.65, resp.) is not observed because of steric hindrance preventing the coplanarity of the mol. and thus limiting the mesomeric forms of the mols. to 2 basic contributing structures. For similar reasons VII, VIII, and X do not show any bathochromic effect as compared with the unsubstituted compd. (λmax. 400 mμ, log ε 4.48). In VII-EtI the quaternization favors 2 contributing structures with either one of the 2 N bearing the pos. charge and causes a hypsochromic effect (λmax. 486 mμ) as compared with the unsubstituted analog (λmax. 524 mμ, log ε 4.60).
IT 875846-34-7, 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)- (derivs.)
RN 875846-34-7 CAPLUS
CN 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)- (5CI) (CA INDEX NAME)

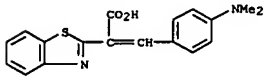


L4 ANSWER 248 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1952:26032 CAPLUS
DOCUMENT NUMBER: 46:26032
ORIGINAL REFERENCE NO.: 46:4402g-i,4403a-d
TITLE: Cyanine and styryl dyes
INVENTOR(S): van Dormael, Andre Emile; de Smet, Polydoor
PATENT ASSIGNEE(S): Gevaert Photo-Producten N. V.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 656515		19510822	GB 1947-8961	19470402

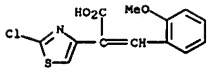
AB New monomethine cyanine and styryl dyes or their cyclammonium salts which are good photographic sensitizers or supersensitizers are prepared Thus 2-(benzoylmethyl)thiazole 2.4 g. is refluxed with p-Me2NC6H4CHO (I) 1.5 g. in AcOH 5 cc., for 2 hrs. Bright yellow crystals are obtained which give a supersensitizing effect with carbocyanine dyes. 5-Acetylmethyl-3-phenyl-1,2,4-oxadiazole and I give bright yellow crystals which supersensitize emulsions in the presence of a 2,2'-cyanine dye (Ia) with a maximum at 575-80 mμ. Et 2-benzothiazole-pyruvate and I give bright yellow crystals which super sensitize Ag emulsions in the presence of Ia with a maximum at 575-80 mμ. Et 2-benzothiazoleacetate (II) and I give bright yellow crystals which supersensitizes Ag emulsions over a broad range even beyond 600 mμ with a maximum at 460 and 570 mμ in presence of Ia, supersensitizes over a broad range to 620 mμ with a maximum at 560 mμ in presence of styryl dyes and shows a strong mutual supersensitizing effect to about 540 mμ in the presence of a compound prepared from 2-[2-(acetylanilino)vinyl]benzoxazole-EtI and p-(diethylamino)aniline sulfate in pyridine and m. 204-5°. II and 2-(methylmercapto)benzothiazole dimethyl sulfate (III) and Et3N give bright yellow crystals which supersensitize Ag emulsions in the presence of Ia with a maximum at 575 mμ. 2-Benzothiazoleacetanilide (IV) and I give bright yellow crystals which are supersensitizers in the presence of Ia with a maximum at 580 mμ. IV is prepared from II and aniline in the presence of pyridine; it m. 159-60°. Benzyl 2-benzothiazoleacetate (V) and I give crystals, m. 142-3°. In the presence of Ia it is a supersensitizer with a maximum at 580 mμ. V is a brownish oil which is prepared from o-aminothiophenol and benzyl cyanoacetate or ethyl benzyl malonate (VI). VI is prepared from K ethyl malonate and BzBr, it m. 197.0-9.5°. 2-Benzothiazoleacetamide (VII) and III give yellow crystals, m. 181.0-1.5°. It is a strong sensitizer for Ag emulsions up to 485 mμ. VII is prepared from ethyl 2-benzothiazoleacetate and NH4OH. Long, colorless needles are obtained, m. 171-2°. Ethyl 4-quinolineacetate and I give yellow needles, m. 135-6°. It is a strong supersensitizer for Ia with a maximum at 575 mμ. 2-(α-Phenylcarbamyl-p-dimethylaminostyryl)-benzothiazole and MeI give a dye, m. 178-80° (with decomposition). It is a supersensitizer for Ia. 2-Benzothiazolethioacetanilide (VIII) and I with piperidine give orange-yellow needles, m. 236.5-7.0°. It is a sensitizer of Ag emulsions up to 550 mμ with a broad maximum at 485 mμ. With Ia it has a maximum at 575 mμ. VIII is prepared from 2-benzothiazoleacetanilide and P2S5 in pyridine, it m. 168-72°.

L4 ANSWER 248 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Anisaldehyde and II with ZnCl2 give a dye m. 147-9°; it is a supersensitizer for Ia. Reaction of II and N,N'-pentamethylene-bis[2-(methylmercapto)benzothiazole bromide) with Et3N give a sensitizer, m. 148-50°, for Ag emulsions up to 485 mμ.
IT 875846-34-7, 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)-
(esters)
RN 875846-34-7 CAPLUS
CN 2-Benzothiazoleacetic acid, α-(p-dimethylaminobenzylidene)- (5CI) (CA INDEX NAME)

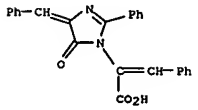


L4 ANSWER 249 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1950:52131 CAPLUS
DOCUMENT NUMBER: 44:52131
ORIGINAL REFERENCE NO.: 44:9960f-i,9961a-b
TITLE: Bromination of 3-acetocoumarin
AUTHOR(S): Koelsch, C. F.
CORPORATE SOURCE: Univ. of Minnesota, Minneapolis
SOURCE: Journal of the American Chemical Society (1950), 72, 2993-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Rap [Gazz. chim. ital. 27, II, 500 (1897)] reported that 3-acetylcoumarin (I) with Br yielded 3-acetyl-4-bromocoumarin; this compound is now shown to be 3-(bromoacetyl)coumarin (II). I (47 g.) in 200 ml. CHCl3, treated with 40 g. Br in 25 ml. CHCl3 (intermittent shaking and warming), and heated 15 min. on the water bath, gives 51-9 g. II, m. 163-5°. II (2.7 g.) in 15 ml. hot EtOH, with 1.6 g. CS(NH2)2 gives (after boiling with H2O containing AcONa) 2.2 g. 2-amino-4-(3-coumarinyl)thiazole (III), bright yellow, m. 225-7°. III (18 g.), 100 ml. AcOH, 200 ml. concentrated HCl, and 40 ml. BuNO2, mixed at 15° and kept 12 hrs. at room temperature, give 9.5 g. 2-chloro-4-(3-coumarinyl)thiazole (IV), m. 170-1°; 1 g. IV, warmed 10 min. with 5 ml. piperidine, gives 0.9 g. 4-(3-coumarinyl)-2-(1-piperidyl)thiazole, deep yellow, b15 310-15°, m. 132-3°; IV and PhNH2 give a gelatinous compound which with Ac2O yields 2-(N-acetylanilino)-4-(3-coumarinyl)thiazole, yellow, m. 230-1°. IV (4.7 g.) and 2.5 g. NaOH in 10 ml. EtOH and 25 ml. H2O, boiled 5 min. and treated with Me2SO4 and NaOH, give 3.2 g. α-(2-chloro-4-thiazolyl)-o-methoxycinnamic acid (V), pale yellow, m. 142-3°; 1.5 g. V and 0.3 g. Na2CO3 in 10 ml. H2O at 20°, treated with 70 ml. 4% KMnO4, give about 200 mg. o-MeOC6H4CHO and 400 mg. 2-chloro-4-thiazolecarboxylic acid, m. 220-1° (decomposition). II (2.7 g.) and 2 g. PhNH2 in 15 ml. EtOH, boiled 15 min., give 2.6 g. 3-(anilinoacetyl)coumarin, red, m. 180-5° (decomposition); Ac derivative, pale yellow, m. 181-2°. II (8 g.) in 100 ml. hot PhMe, treated with 2.5 g. C5H5N and kept 4 hrs. at room temperature, gives 9.7 g. 1-[2-(3-coumarinyl)-2-oxoethyl]pyridinium bromide (VI), pale yellow, decompose about 218°; NaOH gives a gelatinous precipitate which dries to scales resembling Fe(OH)3; the 2-Me derivative (VII) of VI, yellow brown, decompose about 200°; quinolinium analog of VI, orange-brown, decompose about 210°. 3-Carbethoxy-1-[2-(3-coumarinyl)-2-oxoethyl]pyridinium bromide, decompose about 190°; 4-carbethoxy isomer, decompose about 170°.
IT 859479-01-9P, 4-Thiazoleacetic acid, 2-chloro-α-o-methoxybenzylidene-
RL: PREP (Preparation)
(preparation of)
RN 859479-01-9 CAPLUS
CN 4-Thiazoleacetic acid, 2-chloro-α-o-methoxybenzylidene- (5CI) (CA INDEX NAME)

L4 ANSWER 249 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

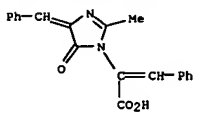


L4 ANSWER 250 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1944:8262 CAPLUS
DOCUMENT NUMBER: 38:8262
ORIGINAL REFERENCE NO.: 38:1210a-e
TITLE: Anhydrides of peptides and dehydrogenated peptides
AUTHOR(S): Tietzman, Josephine E.; Doherty, David G.; Bergmann, Max
SOURCE: Journal of Biological Chemistry (1943), 151, 387-94
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB By heating 20 g. of AcNHC(:CHPh)CONHC(:CHPh)CO2H (I) with 40 ml. of H2O and C5H5N for 4 hrs. at 90°, 8 g. of anhydro-I (II) m. 210-12°, was obtained. Reduction of II by H and Pd gave AcNHCH(CH2Ph)CONHCH(CH2Ph)CO2H, m. 245-6°, and a compound C20H20O3N2, m. 199-200°, Me ester, 135-7°, probably O.CMe:N.CH(CH2Ph).C:NCH(CH2Ph)CO2H, an anhydro peptide. It is not affected by solution at room temperature for 24 hrs. in H2O, N HCl, or NaHCO3. An attempt to prepare an anhydro peptide from AcNHC(:CHPh)CONHCH2CO2H (II) by heating in vacuo at 180° (Graenacher, C. A. 21, 1813) gave only tar. The C5H5N-H2O procedure used above failed to convert either II or the Bz derivative to an anhydro peptide. In the reaction between BzH and NH2CH2CO2H, a compound C20H16N2O3 (III), m. 256° (decomposition), was isolated in addition to the azlactone and polymeric benzylidineglycine (Dakin, C. A. 23, 4205). With NH4OAc, III gave an NH4 salt, and is possibly O.CMe:N.C(:CHPh).C:NC(:CHPh)CO2H. The azlactone of BzNHC(:CHPh)CONHC(:CHPh)CO2H (IV) (C. A. 38, 64.1) on treatment with C5H5N-H2O gave anydro-IV, m. 258-9° (decomposition). The action of N NaOH on AcNHC(:CHPh)CONHC(:CHPh)C:N.C(:CHPh).C(:O).O at room temperature gave an anhydro peptide, probably NH.C(:CHPh).CO.N.C(:CHPh).C:N.C(:CHPh)C:O m. 289° (decomposition)
IT 855164-67-9P, Cinnamic acid, α-(4-benzylidene-4,5-dihydro-5-oxo-2-phenyl-1-imidazolyl)- 855164-69-1P, Cinnamic acid, α-(4-benzylidene-4,5-dihydro-2-methyl-5-oxo-1-imidazolyl)-
RL: PREP (Preparation)
(preparation of)
RN 855164-67-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



RN 855164-69-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

L4 ANSWER 250 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 251 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1943:14515 CAPLUS
DOCUMENT NUMBER: 37:14515
ORIGINAL REFERENCE NO.: 37:2371i,2372a-c
TITLE: Condensation of 2-furanacetic acid with o-nitrobenzaldehyde
AUTHOR(S): Amstutz, E. D.; Spitzmiller, Ervin R.
SOURCE: Journal of the American Chemical Society (1943), 65, 367-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

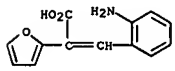
AB K 2-furanacetate (16.5 g.), added to 15.1 g. o-O2NC6H4CHO in 180 cc. Ac2O, the mixture heated at 75° for 12 h. (1 h. to temperature), the solution poured into 300 cc. H2O and neutralized with solid Na2CO3, 400 cc. H2O added, the solution filtered to free it from the insol. tarry substances and acidified, gives 26 g. of a dark green to yellow-brown product; dispersion in boiling H2O gives a solution of trans-α-2-furyl-o-nitrocinnamic acid (I), bright yellow, m. 137.6-8.2° (m. ps. corrected), and as a residue the cis-isomer (II), m. 192-2.4°; the yields were 23.2 and 42.6%. I (450 mg.) in 10 cc. PhNO2 and a crystal of iodine, heated at 210° for 40 min., gives 58% of II; after 20 min., the conversion was about 40%.

I heated with Cu chromite in quinoline gives 15% of trans-o-nitrophenyl-2-furylethylene (III), pale yellow, m. 92.8-3.6°; II (4 g.) gives 2 g. of the cis-isomer (IV), a light brown liquid, b3 152-4°, which did not crystallize. III heated in quinoline for 10 h. at 230° gives a small quantity of a light yellow compound, which was not identified as IV.

Reduction of I by FeSO4 in dilute NH4OH gives 78% of α-2-furyl-o-aminocinnamic acid (V), salmon-yellow, m. 156°; in sunlight it is changed to a tan-yellow. Attempted Pschorr ring closures on V were unsuccessful.

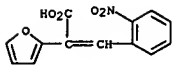
IT 855165-01-4P, Cinnamic acid, o-amino-α-2-furyl-
859999-37-4P, Cinnamic acid, α-2-furyl-o-nitro-, cis-
RL: PREP (Preparation)
(preparation of)

RN 855165-01-4 CAPLUS
CN Cinnamic acid, o-amino-α-2-furyl- (4CI) (CA INDEX NAME)



RN 859999-37-4 CAPLUS
CN 2-Furanacetic acid, α-(o-nitrobenzylidene)- (4CI) (CA INDEX NAME)

L4 ANSWER 251 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 252 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1942:33209 CAPLUS
DOCUMENT NUMBER: 36:33209
ORIGINAL REFERENCE NO.: 36:5175e-i
TITLE: 3-Pyridineacetic acid (β-homonicotinic acid)
AUTHOR(S): Hartmann, Max; Bosshard, Werner
SOURCE: Helvetica Chimica Acta (1941), 24, 28-35E
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 36:33209

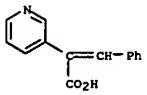
AB A simple method for the production of the previously unknown 3-pyridineacetic acid (I) is described. 3-Pyridyl Me ketone (13 g.) in 100 cc. aqueous (NH4)2S and 10 g. S in 80 cc. dioxane were autoclaved for 6 hrs. at 160-70°. The reaction product was evaporated to dryness in vacuo. The residue was extracted with H2O and the extract was taken down to dryness. Crystallization from alc. by the addition of ether gave 3-pyridineacetamide (II), C7H8N2O, m. 123°. Refluxing 30 g. of crude residue with 300 cc. MeOH in the presence of HCl for 3 hrs. gave Me 3-pyridineacetate (III), b10 112°, hydrolyzed in 10% KOH in MeOH to I, C7H7NO2, m. 144°; Et ester, b12 124°; diethylamide, b12 175°.

III (7.65 g.) in 20 cc. absolute alc. and 20 cc. AcOH was catalytically reduced in the presence of 0.5 g. PtO2. Distillation of the product yielded an acetate (IV), b12 114°, dissociated by steam to Me 3-piperidineacetate, C10H19NO4, which, when recrystd. from a mixture of MeOH and acetone, in. 115-18°. A mixture of 1.0 g. IV in 1 cc. H2O, 0.5 g. of 85% HCO2H and 0.7 cc. of 40% HCHO was heated for 2 hrs. on the steam bath and then evaporated to dryness in vacuo. Esterification of the oily product gave 0.62 g. of Me 1-methyl-3-piperidineacetate, b13 96°, also produced by the catalytic reduction of the Me2SO4 compound of III, and yielding a picrate, m. 112-15°. The MeI derivative from 3.1 g. III was shaken with Ag2O (from 4 g. AgNO3) for 20 hrs. Working up gave the extremely hygroscopic 3-pyridineacetic acid methylbetaine, C8H9NO2, m. 130-2° (decomposition); HCl salt, m. 167° (decomposition); picrate, m. 154-6°. Boiling 10 g. III with 1.5 g. Na and 3.4 g. BzH in 30 cc. absolute ether for 20 hrs., treatment with 65 cc. N HCl and extraction with ether gave an oily ester, b0.2 157°, saponified to α-[3-pyridyl]cinnamic acid, C14H11NO2, m. 233° (decomposition) on recrystn. from alc.

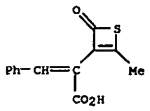
IT 32967-19-4P, 3-Pyridineacetic acid, α-benzylidene-
RL: PREP (Preparation)
(preparation of)

RN 32967-19-4 CAPLUS
CN 3-Pyridineacetic acid, α-(phenylmethylene)- (9CI) (CA INDEX NAME)

L4 ANSWER 252 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 253 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1939:54165 CAPLUS
DOCUMENT NUMBER: 33:54165
ORIGINAL REFERENCE NO.: 33:7779f-i
TITLE: Preparation of thiophene derivatives from ethyl β- carbethoxylevulinate
AUTHOR(S): Mitra, S.; Chakrabarty, N. K.; Mitra, S. K.
SOURCE: Journal of the Chemical Society (1939) 1116-17
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Ac(EtO2C)- CHCH2CO2Et, dissolved in an alc. previously saturated with HCl at
0° and treated with H2S for 12 hrs., gives the ethers of Et 5-hydroxy-2-methylthiophene-3-carboxylate: Me, b5 125°; Et, greenish yellow, b5 150°; Pr, yellow, b5 135°; refluxing with 10% Ba(OH)2 for 4-6 hrs. gives the free acids: 5-methoxy-2-methylthiophene-3-carboxylic acid (I), m. 128°; 5-EtO analog (II), m. 122° (Ba salt, needles); 5-PrO analog (III), m. 75°. II and BzH with EtOH-HCl (1 hr. at 0°) give di(5-ethoxy-3-carboxy-2-methylthienyl)phenylmethane (IV), m. 233°; vanillin gives the 4'-hydroxy-3'-methoxy derivative of IV, m. 235°; III and BzH give the PrO analog of IV, m. 232° (decomposition), and I gives the MeO analog, m. 250° (decomposition). I or II with HBr (mixed at 0° and allowed to stand at room temperature for 1 hr.) gives 5-hydroxy-2-methylthiophene-3- carboxylic acid (V), m. 160°; FeCl3 gives an intense pink color. V and BzH give with EtOH-HCl at room temperature for 1 hr.
5-keto-4-benzylidene-2-methyl-4,5-dihydrothioph.acte.ine-3- carboxylic acid, bright yellow, m. 166°; 4-o-nitrobenzylidene analog, bluish yellow, m. 184° (decomposition); 4- methoxybenzylidene analog, brilliant orange-yellow, m. 152°. V and AcH give the 4-ethylidene compound, hay- colored, m. 124°; cinnamaldehyde gives the 4-cinnamylidene compound, orange, m. 204°.
IT 858807-09-7P, Succinic acid, α-benzylidene-β-1-mercaptoethylidene-, thio lactone
RL: PREP (Preparation)
(preparation of)
RN 858807-09-7 CAPLUS
CN Succinic acid, α-benzylidene-β-1-mercaptoethylidene-, thio lactone (4CI) . (CA INDEX NAME)



L4 ANSWER 254 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1935:1109 CAPLUS
DOCUMENT NUMBER: 29:1109
ORIGINAL REFERENCE NO.: 29:135h-i,136a-g
TITLE: Certain reactions of Γ-ketonic acids
AUTHOR(S): Allen, C. F. H.; Normington, J. B.; Wilson, C. V.
SOURCE: Can. J. Research (1934), 11, 382-94
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 27, 2143. The following chalcones and derivs. are described: 2'-chloro-5'-methyl, b6 195-200°; dibromide, m. 117°; 2'-methyl-5'-isopropyl, b12 205-10°; dibromide, m. 140-1°; 3,4-methylenedioxy-4'-chloro, m. 128°; 4'-fluoro, m. 76-7°; 2',4',6'-tri-methylchalcone dibromide, m. 131°. 3,4-Methylenedioxy-benzoyl-p-chlorobenzoylmethane, m. 151°; benzoylmesitoyl-methane (mesitoyl = 2,4,6-Me3C6H2CO), m. 84°; 3-p-chlorobenzoyl-5-piperonylisoxazole, m. 180°; 3-mesityl-5-phenylisoxazole, m. 76°; α-bromobenzal-2,4,6-trimethylacetophenone, m. 73°. The following nitriles, corresponding acids and esters of the α-aryl-β-aroyl propionic acid series were prepared: α-phenyl-β-(4-fluorobenzoyl)-propionitrile, m. 102°; acid, m. 161°; Me ester, 101°; α-phenyl-β-(4-phenylbenzoyl)propionitrile, m. 176°; Me ester, m. 157°; α-phenyl-β-(p-toluyl)propionitrile, m. 80°; acid, m. 152°; Me ester, 112°; α-phenyl-β-(4-nitrobenzoyl)propionitrile, m. 155°; Me ester, m. 104°; α-phenyl-β-(4-carboxybenzoyl)propionitrile, m. 239°; di-Me ester, m. 110°; α-phenyl-β-(2-chloro-5-methylbenzoyl)propionitrile, m. 76-7°; Me ester, m. 80°; α-phenyl-β-mesitoylpropionitrile, m. 77-8°; acid, m. 172°; Me ester, m. 60-1°; α-piperonyl-β-(4-chlorobenzoyl)propionitrile, m. 129°; acid, m. 190°; Me ester, 109°; α-phenyl-β-(4-bromobenzoyl)propionic acid, m. 160°; Me α-piperonyl-β-benzoylpropionate, m. 121°; β-(4-chlorobenzoyl)propionic acid, m. 131°; Me ester, m. 63°; β-mesitoylpropionic acid, m. 107°. The following lactols (ketonic acids), derivs. of acrylic acid, are described: α-phenyl-β-benzyl-β-mesitoyl, m. 250° (decomposition); α-piperonyl-β-benzyl-β-(4-chlorobenzoyl), m. 153°; p-bromoanilide, m. 176°; α-piperonyl-β-benzyl-β-benzoyl, m. 138°; α-phenyl-β-benzyl-β-(4-phenylbenzoyl), m. 144°; chloride, m. 150°; α-phenyl-β-benzyl-β-(p-toluyl), m. 133°; α-phenyl-β-benzyl-β-(4-carboxybenzoyl), m. 240°; Me ester, m. 137°; chloride, m. 197°; α-phenyl-β-(2-chlorobenzyl)-β-(4-chlorobenzoyl), m. 147°; α-anisyl-β-(2-methoxybenzyl)-β-benzoyl, m. 126°; α-phenyl-β-(2-chlorobenzyl)-β-benzoyl, m. 98°; α-anisyl-β-(2-chlorobenzyl)-β-benzoyl, m. 154°; α-anisyl-β-(α-furylmethyl)-β-benzoyl, m. 121°. The highly substituted acrylic acids were treated with the Grignard reagent to differentiate between the 2 possible structures (lactol or open-chain acid). AcCl was found to be a satisfactory confirmatory reagent, giving chlorides with the lactols but not with the open-chain acids. From the available evidence it is concluded that the differences may be attributed to cis-trans isomerism. The α-aryl-β-aroyl propionic acids and the β-aroyl propionic acids were investigated with both reagents. The Grignard reagent

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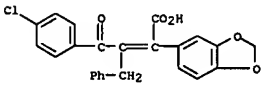
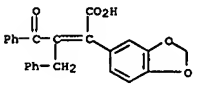
indicated mostly open-chain structures. The use of AcCl led to a variety of products; by varying the procedure, dimers of undetd. structure, unsaturated ketones, enolic acetates and Me esters were obtained. α-Phenyl-β-(p-chlorobenzoyl)propionic acid with AcCl gives C32H24O5Cl2, m. 235° (decompn.). α-Phenyl-β-mesitoylpropionic acid with AcCl yields a crotolactone, m. 126°, and a substance of high m. p. α-Phenyl-β-benzyl-β-(4-chlorobenzoyl)-propionic acid, m. 173-4°, is formed by the reduction of the corresponding acrylic acid. β-(p-Chlorobenzoyl)propionic acid and AcCl give Γ-(p-chlorophenylcrotolactone). Similarly β-mesitoylpropionic acid gives a compd., C26H2404, (Pechmann dye?) and the enol-acetate. CH2.(CH2)4.C:O with AcCl gives the acetate. The mechanism of the reactions is discussed,
as well as evidence for the possible structures of derivs. of Ac(CH2)2CO2H. A mechanism is suggested for the formation of enolic esters
and unsatd. lactones of enolized ketonic acids. Numerous tables of results are included.
IT 857828-53-6P, Crotonic acid, β-p-chlorobenzoyl-α-(3,4-methylenedioxyphenyl)-γ-phenyl- 857828-67-2P, Crotonic acid, β-benzoyl-α-(3,4-methylenedioxypheny1)-γ-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 857828-53-6 CAPLUS
CN Crotonic acid, β-p-chlorobenzoyl-α-(3,4-methylenedioxyphenyl)-γ-phenyl- (3CI) (CA INDEX NAME)

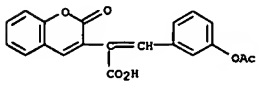


RN 857828-67-2 CAPLUS
CN Crotonic acid, β-benzoyl-α-(3,4-methylenedioxyphenyl)-γ-phenyl- (3CI) (CA INDEX NAME)

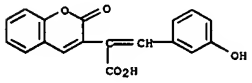


L4 ANSWER 255 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1934:50529 CAPLUS
DOCUMENT NUMBER: 28:50529
ORIGINAL REFERENCE NO.: 28:6131i,6132a-f
TITLE: Reactivity of the methylene group in coumarin-3-acetic acids. Condensation with aromatic aldehydes
AUTHOR(S): Dey, B. B.; Sankaranarayanan, Y.
SOURCE: J. Indian Chem. Soc. (1934), 11, 381-7
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 26, 3499. A comparison of the activities of the CH2 groups in PhCH2CO2H and coumarin-4-acetic acids has shown the latter to be more reactive. It may be argued that the activity of this group in coumarin-3-acetic acids is lower than that in the 4-acetic acids since, while the latter and their Et esters condensed easily with aldehydes under the conditions of both the Perkin and Knoevenagel reactions, coumarin-3-acetic acids (I) can only be made to react by Perkin's method. A mixture of the Na salt of I (3 g.), freshly distilled BzH (1.4 g.) and 12 g. of Ac2O was refluxed at 160° for 5 hrs. The product was decomposed by boiling in H2O and yielded 1.4 g. of phenyl-3-coumarylethylenecarboxylic acid, m. 202°. A similar condensation with p-HOC6H4CHO gave a solid product which dissolved in contact with dilute alkali, leaving a residue (II). Acidification of the solution gave p-acetoxyphenyl-3-coumarylethylenecarboxylic acid (III), m. 244°. Repeated recrystn. of II produced p-acetoxyphenyl-3-coumarylethylene (IV), m. 165°. Hydrolysis of III and IV by boiling with 2.0 N NaOH for 30 min. yielded the corresponding p-HO compds., m. 272° and 227°, resp. In contrast with the behavior of the 4-acetic acids which yielded only coumarinphenylethylenes by the Perkin reaction the condensation products from the 3-acetic acids consist mainly of the ethylenecarboxylic acids, existing chiefly in the form of the saturated lactones which are sufficiently stable to resist the action of Na2CO3 but which are converted by alkali into the salts of the free acids, from the solns. of which the original lactones are repptd. on acidification. The alternative view that the action of alkalies entails a fission of the pyrone and not of the new lactone ring is equally plausible. The following compds. were prepared by condensing coumarin-3-acetic acids with various aldehydes: 3-coumarylethylene-carboxylic acids; m-acetoxyphenyl (V), m. 188° (hydrolyzed to the m-HO compound, m. 242°); 3-methoxy-4'-acetoxyphenyl, m. 207° (hydrolyzed to 3'-methoxy-4'-hydroxyphenyl, m. 211°), 4'-methoxyphenyl, m. 225°, 3',4'-methylenedioxyphenyl, m. 270°, βα-naphtho-3-coumarylphenylethylenecarboxylic acid, m. 253°, 7-acetoxy-4-methyl-3-coumaryl-3'-coumarin, m. 268°, 7,7'-diacetoxy-4-methyl-3,3'-bicoumarin, m. 220°, 7-acetoxy-4-methyl-3-coumaryl-3'-βα-1,2-naphthopyrone, m. 272°, 3,3'-bi-βα-naphthopyrone, m. 345°, and the 3-coumarylethylenes, m-acetoxyphenyl, m. 140°, the by-product in the preparation of V, and its hydrolysis product m-hydroxylphenyl, m. 193°. The products of condensation of p-HOC6H4CHO and vanillin

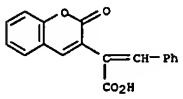
L4 ANSWER 255 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto-, acetate (3CI) (CA INDEX NAME)



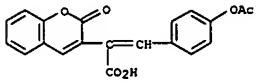
RN 876498-00-9 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto- (3CI) (CA INDEX NAME)



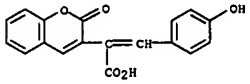
L4 ANSWER 255 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
with I exhibit the same color changes when treated with alkali as the analogous products derived from the 4-acetic acids. They are assumed to tautomerize readily, in the presence of alkalies, into quinonoid forms which, however, revert to the normal structure through opening of the pyrone ring by prolonged contact with alkali.
IT 860564-98-3P, 1,2-Benzopyran-3-acetic acid, α-benzal-2-keto- 872276-36-3P, 1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto-, acetate 876497-98-2P, 1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto- 876497-99-3P, 1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto-, acetate 876498-00-9P, 1,2-Benzopyran-3-acetic acid, α-[m-hydroxybenzal]-2-keto-
RL: PREP (Preparation)
(preparation of)
RN 860564-98-3 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-benzal-2-keto- (3CI) (CA INDEX NAME)



RN 872276-36-3 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto-, acetate (3CI) (CA INDEX NAME)



RN 876497-98-2 CAPLUS
CN 1,2-Benzopyran-3-acetic acid, α-[p-hydroxybenzal]-2-keto- (3CI) (CA INDEX NAME)



RN 876497-99-3 CAPLUS

L4 ANSWER 256 OF 256 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1931:32742 CAPLUS
DOCUMENT NUMBER: 25:32742
ORIGINAL REFERENCE NO.: 25:3653g-i
TITLE: Synthesis of 4-methoxy-6,7-methylenedioxyphenanthrene and 4-methoxy-5,6-methylenedioxy-9-phenanthrenecarboxylic acid
AUTHOR(S): Girardet, A.
SOURCE: Helvetica Chimica Acta (1931), 14, 513-5
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The condensation of 18 g. of 3,4-(CH2O2)C6H3CH2CO2H (C. A. 18, 3385) with 18.1 g. of 2,3-O2N(MeO)-C6H3CHO (Ber. 28, 1385(1895)), in the presence of Ac2O and SnCl2 gave 18.5 g. of α-3,4-methylenedioxyphenyl-β-2-nitro-3-methoxyphenylacrylic acid, m. 225°. This was converted into the corresponding amino derivative, m. 221°, by the aid of NH3-FeSO4. By diazotization in 2 N H2SO4, boiling with mol. Cu and extraction of the cooled solution with Et2O, 4-methoxy-6,7-methylenedioxyphenanthrene-9-carboxylic acid, m. 271°, was formed. This acid was decarboxylated by sudden immersion in a metal bath at 300°, yielding a non-crystalline phenanthrene whose picrate, m. 160-1°, is not identical with that of the methylpukateine derivative By hydrolysis of 6-bromopiperonal azolactone with 10% NaOH and oxidation of the resulting pyruvic acid derivative, 5,6-(CH2O2)C6H3CH2CO2H, m. 192°, was prepared This was condensed with 2,3-O2N(MeO)C6H3CHO, the resulting product being reduced to the amino acid and converted by diazotization and consequent decomposition with mol. Cu into 4-methoxy-5,6-methylenedioxy-8-bromo-9-phenanthrenecarboxylic acid, m. 223°. This acid was debrominated by refluxing with alc. KOH and a Zn-Cu powder. Attempts to decarboxylate the non-brominated acid failed, some of the decomposition products esterifying the unchanged acid.
IT 860582-71-4P, Acrylic acid, α-(3,4-methylenedioxyphenyl)-β-2-nitro-m-anisyl-
RL: PREP (Preparation)
(preparation of)
RN 860582-71-4 CAPLUS
CN Acrylic acid, α-(3,4-methylenedioxyphenyl)-β-2-nitro-m-anisyl- (3CI) (CA INDEX NAME)